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Application of CFAST to Shipboard Fire Modeling III. Guidelines for Users

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The use of the Consolidated Fire Growth and Smoke Transport (CFAST) fire model is well established within the civilian community. In recent years, the U.S. Navy has sponsored enhancements to the model (including the addition of vertical vent flow, corridor flow, and improved heat conduction) to make the model more useful in Navy fire scenarios. This report is the third (and last) in a series that documents the current state of CFAST. The purpose of this report is to provide guidance for the routine application of CFAST in ship design.

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1.0 INTRODUCTION

There are two primary areas in which computer fire modeling could be of benefit to the US Navy. The requirements imposed by these applications are different and, in some ways, complementary. The first application, ship design, requires a capability for performing detailed simulations in a complex environment, but has few restrictions on the time required to obtain results. For the second area, real-time prediction of fire behavior, the model must be able to run faster than real time, but the predictions may be less detailed.

These requirements approximately correspond to the capabilities of the two different classes of fire models: field models and zone models. Field models typically divide the region of interest (domain) into hundreds, thousands or even millions of small volumes (cells), the dimensions of which are typically on the order of centimeters or smaller. Temperature, pressure, species concentrations and other variables are calculated for each cell as a function of time and each variable is represented as a time variant scalar or vector field (hence the name field model). The results of these calculations can be very detailed, both in spatial resolution and in terms of the amount of information available for each cell. However, field models are very slow — it is not unusual to require hours of supercomputer time to simulate fractions of a second of real time, even for physically small systems.

At the other extreme, zone models commonly use only one or two very large homogeneous volumes (zones) to represent a volume that might require hundreds of thousands of cells in a field model. In addition, zone models typically ignore physical and chemical details so that each zone is normally represented by many fewer variables than would be the case in a field model. Finally, zone models usually represent only the time variations of the variables and use ordinary, rather than partial, differential equations. This combination of factors (fewer computational elements, reduced numbers of variables per element and simplified equations for each variable) permits zone models to be many orders of magnitude faster than field models.

Of course, this gain is not free — the trade-offs for increased speed are reduced spatial resolution and lower accuracy of the predictions. For some applications, including real-time prediction over a relatively short time span (perhaps 30 minutes), this is an acceptable compromise and it is reasonable to use a zone model. In other applications, the lower accuracy and resolution are not acceptable and field models must be used. For ship design, it is likely that there will be a role for zone models, especially in the early phases, but that field models will be needed for the detailed design phase.

The Consolidated Fire Growth and Smoke Transport (CFAST) model [1] is an example of the zone model class. Developed over a period of many years by the National Institute of Standards and Technology (NIST), CFAST was designed to provide fast and reasonably accurate predictions of fire and smoke spread in buildings. In recent years, the US Navy has funded improvements in the CFAST model to make it more applicable to shipboard fires. With Navy sponsorship, CFAST has gained capabilities for modeling phenomena that are absent from, or of little significance to, building fires. This has included mass transport through vertical vents (representing hatches and scuttles) [2], energy transport via conduction through decks [3] and improvement to the radiation transport submodel [4]. Work is currently underway at the Naval Research Laboratory (NRL) to validate the most recent addition, horizontal compartment-to-compartment heat conduction through bulkheads.

During the development of CFAST, certain simplifying assumptions (in addition to those which are inherent in zone models) were made regarding the types of phenomena and the complexity of

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the scenarios which were to be modeled. Those assumptions led to limitations on the scope of the problems which can be modeled, the ease with which they can be modeled and the accuracy of the results.

We have already noted that zone models have inherent limitations regarding the level of detail which they can provide and we have alluded to the fact that some physical phenomena have been left out of CFAST in order to simplify the model and permit fast execution. One major area that is absent for CFAST is reaction chemistry — in CFAST, the fire and its combustion products are inputs which must be specified by the user.

In addition, the choice of algorithms and the manner in which they have been implemented impose certain limitations. For example, all compartment surfaces were assumed to be rectangles and this assumption is embedded in the code at every point that an area or volume is calculated. In other cases, the function used to represent a phenomenon was based on correlations with experiments (rather than on first principles) and is only valid for the range within which the experiments were performed.

In the case of building fires, these limitations have not been unduly restrictive but, due to significant differences between Navy and civilian fire protection problems, the impact of CFAST limitations for the Navy has not been known. To address that question, the Office of Naval Research sponsored an NRL project, "Analysis of the CFAST Fire Model Operating Envelope," to identify CFAST limitations, determine their effects on shipboard fire modeling and, where necessary, to develop methods for circumventing those problems.

Our approach to this task was to apply CFAST to modeling of a full-scale shipboard fire test and then to compare the model predictions with the test data. For this case study, we selected test 4_10 from the Submarine Ventilation Doctrine [5] program. That test was conducted, during January 1996, in the SHADWELL/688 test area (Figure 1) aboard the ex-USS SHADWELL. This configuration represented the forward half of a USS LOS ANGELES (SSN 688) class submarine.

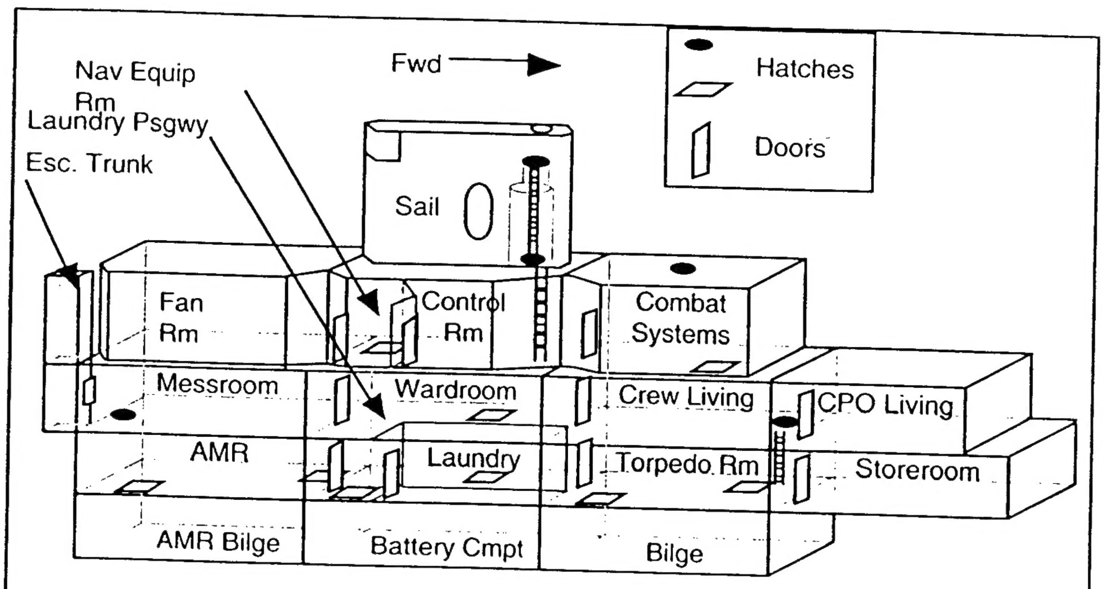

Figure 1. SHADWELL/688 Test Area

Test 4_10 was selected for study because, for that case, the fire was located in the Laundry Room and the mechanical ventilation ducts were sealed. Having the fire in the Laundry Room was

important because that was the least complex compartment (it was a rectangular parallelepiped) and allowed us to simulate the fire without the confounding factor of geometric complexity. The fact that the ventilation ducts were sealed significantly reduced the difficulty of the problem, since we only had to contend with buoyancy flows through hatches and doors.

The work proceeded in two phases. In the first, we developed the fire specification and tested it against Laundry Room data [6]. During the second phase, the original model was extended by sequentially adding surrounding compartments while keeping the fire specification unchanged [7]. In order to minimize bias due to foreknowledge of the actual test outcomes, the test results were not used in either phase until after the modeling was completed[1], at which time the model predictions were compared with test results to determine the accuracy of the model. CFAST version 3.1.4[2], was used for this project.

The purpose of this report is to summarize the findings from both phases and to present them in a form which will be useful to engineers or designers interested in applying CFAST to shipboard fire problems.

2.0 CFAST BASICS

In this report, we discuss, in the form of a case study, the application of CFAST to problems of Navy interest. In particular, we focus on the problems that were encountered and the solutions which were developed during modeling of a portion of the ex-USS SHADWELL. We start with a discussion of the basics of using CFAST but make no attempt to replicate the material in the definitive CFAST references, which are the NIST user guide [8] and technical reference [9]. The former discusses CFAST from the perspective of someone who simply wants to use CFAST as a tool while the latter provides an explanation of the underlying methodology and algorithms and is primarily of scientific interest.

2.1 The CFAST Input File

The execution of a CFAST model is controlled by a text input file which contains all of the information required to describe the desired simulation. Each piece of information appears as a parameter associated with a keyword. Collectively, the keywords and corresponding parameters constitute the vocabulary of the CFAST command language. This implies the existence of another class of limitations, in addition to those previously mentioned, because no problem can be simulated unless it can be described using the CFAST vocabulary. We will encounter several instances which illustrate this problem.

Some keywords have only a single associated parameter, others have several parameters and still others may have a variable number. Except for comment lines, which begin with the pound sign (#) and are ignored by CFAST, a keyword appears at the beginning of each line in the command file. Keywords may be included in any order and, where appropriate, the parameters associated with a keyword appearing later in the file will replace values that appeared earlier.

For the following discussion, we divide the keywords into four categories: (1) simulation control; (2) ambient environment; (3) model geometry and (4) fire description. The keywords which we

[1] There were two exceptions to this rule. First, the measured fuel mass loss rate was given as an input to CFAST to ensure that we simulated the specific fire that was present in test 4_10 and, second, we used an experimental value for the CFAST carbon monoxide production parameter. The latter was done only after it was determined that the carbon monoxide parameter had no significant effect on temperature predictions. Further details may be found in reference [6].

[2] Subsequent to the date of this work, CFAST Version 4 was released for public use. The major new feature of Version 4, horizontal heat conduction, has not yet been validated against experimental data.

used in our work are briefly described in Appendix A but that is not an exhaustive list. Further information may be found in reference [8].

2.1.1 Simulation control keywords

Keywords in this category (see Table A-1) affect the manner in which the fire simulation is executed. They include the CFAST version (VERSN), the simulation time (TIMES), the name of the output data file (DUMPR) and the time base for events (FTIME). Listing 1 shows an example of the use of these keywords. The RESTR keyword was not used in this work, but provides a mechanism by which a simulation may be restarted from the results of a previous run.

```
VERSN     3 SHADWELL/688 Laundry - Sail.
#         Sim.time  Print  Hist.  Disp.  Copies
TIMES       1250      1      3      0      0
#                    t0     t1
FTIME                      1250.
DUMPR model.HI
```

Listing 1. Examples of the CFAST Simulation Control Keywords.

VERSN indicates the version of CFAST for which the file was created and provides an option for labeling the current simulation. TIMES sets the total simulation time, the interval between on-screen printouts and the interval between dumps to the history file, all in seconds. The last two parameters are the interval between graph updates (in seconds) and the number of hard copies of each graph that should be produced. FTIME defines the times at which events occur and DUMPR specifies the name for the history file.

CFAST reads the major version number (the first character following the VERSN keyword) of the input file and will refuse to run if it is greater than the actual version of CFAST. For example, CFAST 2.x will not execute simulations designed for CFAST 3.x. VERSN also permits the user to specify a descriptive title (up to 50 characters) for the simulation.

The TIMES keyword takes five parameters. The first, simulation time, is the number of seconds that CFAST will simulate and is independent of the actual running time of the model. The latter depends on the speed of the computer and the complexity of the scenario. The second and third parameters allows the user to set the number of (simulated) seconds between screen updates and history file updates, respectively. The last two parameters control the time interval between on-screen graphic display updates and the desired number of hard copies of each graphic display. Rather than use the limited built-in graphics capabilities of CFAST, most users post-process the history file and plot the results off-line.

FTIME is the most important of the simulation control keywords and requires further explanation. CFAST allows the user to define events, such as opening and closing vents or controlling the growth of the fire. Events can occur at user-specified times but there is a single time base that is used by all events. FTIME defines this timeline by listing (in seconds elapsed since the start of the simulation) the time for each event.

For example, suppose we wish to specify a series of events, shown in Figure 2, for vents A and B. At the start of the simulation, vent A is closed and B is open. Vent A opens at time t_1, closes again at time t_2 and then remains closed for the rest of the simulation while vent B stays open until t_3. To achieve this, we first define times t_1 through t_3 using the FTIME keyword and then

specify each of the vent openings (as a fraction of the maximum width[3]) for each of these times, even if there is no change for that vent at that time. This vent sequence is illustrated in Table 1.

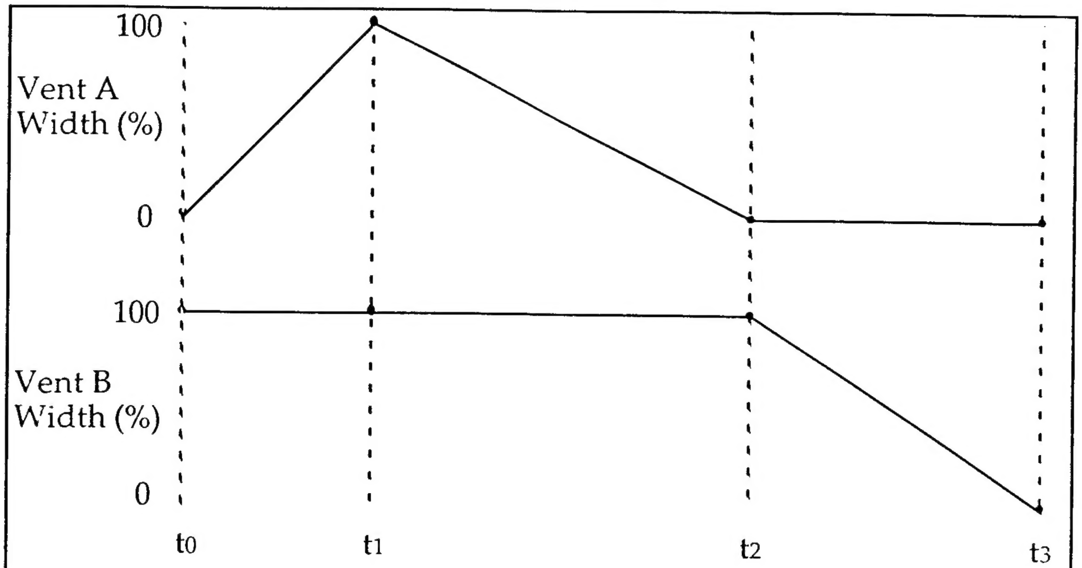

Figure 2. Vent Closure Sequence Example

FTIME		t1	t2	t3
CVENT A	0	1	0	0
CVENT B	1	1	1	0

Table 1. Example of the CFAST Event Mechanism

Events can be triggered at the elapsed times (in seconds) specified by FTIME. In this case, the CVENT commands cause vents A and B to fully open (1) or completely close (0) at times zero, t_1, t_2 and t_3. Note that an event time at zero seconds is implied.

There is an implicit t_0 in FTIME but events must be explicitly provided for all times, including t_0 (*i.e.*, the first event in each set is assumed to occur at t_0, even though zero is not listed in the time line). This is because CFAST reads the events from left to right; the first event is assumed to occur at zero time and subsequent events are sequentially associated with the times listed in the FTIME line. If an event is missing, then the following events will be associated with the wrong time.

Because CFAST uses linear interpolation to calculate values for intermediate times, transitions occur over the period between sequential event times rather than instantaneously. If the transition is too steep (*i.e.*, there is a large change in the parameter value between two closely spaced time points), CFAST may encounter numerical problems and drastically slow down or even stall. If problems of this nature are encountered, it is recommended that the transition be spread over a longer period of time.

[3] CFAST only permits vent widths to be varied. This is appropriate for doors but does not correctly represent vertically opening vents such as windows.

FTIME only affects some keywords — those which permit a list of values to be defined for different times. Values for other keywords cannot be changed using FTIME. However, in principle, any parameter can be altered by using RESTR, which causes CFAST to initialize the simulation to values calculated by a previous simulation. This has the effect of instantly switching from the parameter set associated with the first simulation to that of the second.

This is particularly useful when there is a sudden change in the type of fuel involved. For example, some of the NRL large-scale tests began with a hexane pan fire and switched, virtually instantaneously, to a diesel spray fire. This was modeled by first simulating the pan fire, using parameters characteristic of hexane, up to the time of ignition of the spray fire and then restarting the model with diesel fuel fire parameters.

2.1.2 Ambient environment keywords

The use of two ambient environment keywords (see Table A-2) are illustrated in Listing 2 TAMB indicates the initial conditions within the simulation region; EAMB refers to the exterior conditions. There can only be one instance of each. Note that the requirement that there be only a single TAMB line implies that the entire model domain described by a single initial condition prior to the start of the simulation.

```
#       Temp.     Press.     Elev.
TAMB    285.900   101300.    0.000000
EAMB    286.300   101300.    0.000000
```

Listing 2. Examples of the CFAST Ambient Condition Keywords.

TAMB and EAMB describe the initial temperature and pressure and reference elevation within and outside of the modeling domain, respectively. The reference elevations are the actual elevations (meters above mean sea level) at which the temperatures and pressures were specified.

For each keyword, the temperature (kelvins), pressure (Pascals) and reference elevation (meters above mean sea level) are given. The elevation of the reference point is needed so that the model can correct for altitude-related temperature and pressure changes. Correction for differences in elevation can be important for high-rise buildings, but is not expected to be significant for shipboard fire modeling. The reference elevation can be any convenient point, but the same point must be used for both keywords. The elevation of the lowest compartment is typically used and, for ships, this would normally be zero (sea level).

A third ambient keyword, WIND, permits the user to specify the wind speed, the elevation at which that speed was measured and a coefficient for calculation of wind speeds at other heights. These parameters are only significant if there are high winds that interact with doors, windows or other vents. WIND was not used in this work and is not expected to be important for most naval problems.

2.1.3 Implicit Geometric Limitations

The limitations of the CFAST inputs impose some restrictions on our ability to define complicated geometries. In this section, we will discuss some of these restrictions, including the following:

a. all compartment boundaries are rectangular;

b. each compartment has only a single bulkhead, which wraps around all four sides;

c. for any compartment, the overhead, deck and bulkheads are each limited to a single set of thermophysical properties;

d. vent[4] locations are undefined[5];

e. all horizontal vents are rectangular; and

f. vertical vents must be either circular or square.

The first limitation is due to the fact that the dimensions of each compartment are described by only three parameters: DEPTH, WIDTH and HEIGH. This implies that each compartment is a rectangular parallelepiped, *i.e.*, there are exactly six bounding surfaces, each of which is a rectangle. The deck and overhead are assumed to have identical dimensions and, since there is no provision for defining individual walls, CFAST treats the compartment vertical boundary as one continuous entity[6]. As a corollary, there is no way to specify in which bulkhead a horizontal vent is located.

Also, each boundary has only one associated entry in the thermophysical properties database. Thus, the deck, overhead and the entire wrap-around bulkhead each has only one set of properties — it is not possible to exactly represent compartment boundaries that have patches composed of different materials[7].

These inherent limitations force us to make approximations in order to describe many common shipboard situations. For example:

a. many compartments do not have simple, rectangular cross sections;

b. standard water tight doors are not rectangles; and

c. watertight hatches (except for scuttles) are usually neither square nor circular.

Later in this report we will encounter several instances where approximations were required to circumvent these limitations. Examples of our approximation methods will be presented, along with discussions of the implications of these methods.

2.1.4 Geometry keywords

Examples of the use of the most important geometry keywords (see Table A-3) are given in Listing 3. Compartment floor elevations (meters), relative to the reference point defined by the ambient environment inputs, are given by HI/F and the dimensions of each compartment (meters) are specified using DEPTH, WIDTH and HEIGH. The dimensions of each compartment

---

[4] In CFAST terminology, a vent is any opening between compartments (or between a compartment and the outside), except for ventilation ducts, which have their own special set of keywords. Since we did not use ventilation ducts in these simulations, references to vents appearing in this report refer to doors, windows, hatches, scuttles and similar openings. An oddity of CFAST nomenclature is that vents are described by the direction of the flow through the vent, not by the orientation of the vent itself. For example, a door is a horizontal vent, because it allows horizontal flow, although the orientation of the door is vertical. Hatches and scuttles permit vertical flow and are classified as vertical vents.

[5] For an exception to this rule, see the discussion of the HALL keyword in section 2.1.4.

[6] For each time step, CFAST divides the wall into upper and lower portions and independently calculates values for the state of each portion.

[7] It is possible to specify boundaries composed of multiple layers where each layer may have different properties. For example, a bulkhead could be specified as having a steel core with cork on one side and fiberglass on the other.

are specified in terms of a right-handed Cartesian coordinate system with the origin located at the lower, left rear corner of the compartment.

```
#        Cmpt. 1   Cmpt. 2   Cmpt. 3   Cmpt. 4   Cmpt. 5   Cmpt. 6   Cmpt. 7
#        Laundry   Psgwy     Wardrm    NER       CR        Sail_1    Sail_2
#Floor elevation
HI/F     0.00      0.00      2.57      5.16      5.16      7.75      10.18
DEPTH    1.75      10.26     4.00      2.92      2.90      1.21      0.91
#Y dimen.
WIDTH    6.07      2.22      8.51      1.90      6.30      1.42      0.91
#Z dimen.
HEIGH    2.57      2.57      2.59      2.59      2.59      2.43      1.02
#Materials
CEILI    SHIP3/8   SHIP3/8   SHIP7/8   SHIP3/8   SHIP3/8   SHIP3/8   SHIP3/8
WALLS    SHIPLR    SHIPLRP   SHIPWR    SHIPNER   SHIPCR    SHIP3/8   SHIP3/8
FLOOR    SHIP3/8   SHIP3/8   SHIP3/8   SHIP7/8   SHIP7/8   SHIP3/8   SHIP3/8
#
#Laundry-Passageway door
#        Cmpt#     Cmpt#     Vent#     Width     Soffit    Sill
HVENT    1         2         1         0.66      1.90      0.00
#        Cmpt#     Cmpt#     Vent#     Width@t0  Width@t1
CVENT    1         2         1         1.00      1.00
#Passageway-Wardroom hatch
#        Cmpt#     Cmpt#     Area      Type (1 = circular; 2 = square)
VVENT    2         3         0.78      2
#Laundry-Wardroom heat conduction
#        Cmpt#     Cmpt#
CFCON    1         3
```

Listing 3. Examples of the CFAST Geometry Keywords.

These are the major keywords used to define the geometry for a typical CFAST simulation. HI/F is the compartment floor height (relative to the reference elevation from Listing 2); DEPTH, WIDTH and HEIGH specify the dimensions of the compartments. CELI, WALLS and FLOOR identify the ceiling, wall and floor materials. The actual properties of these materials are contained in a separate database file, THERMAL.DF. HVENT specifies horizontal vents (doors, for example) while CVENT permits vents to be opened or closed during the simulation.

Construction materials used for the ceiling, walls and floor are identified by the keywords CEILI, WALLS and FLOOR, respectively. The parameters for these keywords are the names of the construction materials as they appear in the material property database which is a text file. By default, the file THERMAL.DF is used, but this can be changed by using the THRMF keyword to specify a different filename. The properties database contains the name of the material and a list of thermophysical properties, which include thermal conductivity, specific heat, density, thickness and emissivity. The term "thermophysical properties database" is somewhat misleading because the values apply to a specific thickness of the material. Thus, the database we used included many entries for steel, reflecting the different thicknesses used in various parts of the SHADWELL test area. A standard version of THERMAL.DF is provided with CFAST and may be edited, using any text editor, to include additional materials. The file format is specified in the CFAST User's Guide [8].

Recall that, for each compartment, only one material (including thickness) can be defined for the ceiling, walls or floor. If any boundary of the compartment in question has regions constructed of different materials (or different thicknesses of the same material), then some approximation must

be applied. In a subsequent section of this report, we discuss some methods for making these approximations.

It is important to emphasize that CFAST treats walls as wrap-around entities so that each compartment is surrounded by a single wall, not by four separate walls. Thus, not only is it impossible to exactly model situations where a single wall has regions of different materials, some approximations must also be made in those cases where different walls have different compositions.

Each of the keywords mentioned above (except for THRMF) is followed by a list of values, one value per compartment. Compartment numbers are determined by the order of the parameters, *i.e.,* the first parameter following the keyword applies to compartment one, the next to compartment two and so on. There is no keyword to declare the number of compartments; instead, CFAST determines this value by counting the parameters associated with these keywords. If N parameters are found, CFAST assumes there are N compartments. Furthermore, it also assumes that "compartment" (N+1) refers to the world outside of the model domain.

It is important that the same number of parameters appear in each of these lines. If different numbers appear on different lines of the input file, CFAST will run without reporting any errors but the results, as might be expected, are likely to be erroneous.

HVENT and VVENT are used to define horizontal and vertical vents, respectively. HVENT requires six parameters; in addition, there are three, seldom used, optional parameters. The first two required parameters identify the two compartments that are connected by the vent. As mentioned above, compartment numbers are determined by the order in which their dimensions were declared. Recall that, for an N-compartment simulation, compartment (N+1) represents the ambient environment. This convention allows the definition of vents that connect between a real compartment and the external environment.

CFAST permits up to four HVENTs between the same pair of compartments, so the third HVENT parameter is a number (from one to four) that identifies which particular vent is being defined. The next three parameters specify the vent width, the height of the soffit (top) and the height of sill (bottom), respectively.

The first optional parameter is the cosine of the angle between the wind vector and the vent opening[8]. This is applicable only to vents that connect to the exterior and is meaningful only if a wind speed is declared via the WIND keyword. The last two parameters define the horizontal position of the vent with respect to the origins of the two connected compartments. These parameters, which were recently added to CFAST to permit modeling of flows in long, narrow corridors using the HALL keyword, will not be discussed further because they were not used in our work. Additional information about the HALL keyword may be found in reference [10], which reports on the validation of the new corridor flow algorithm.

Like HVENT, VVENT also requires two parameters to define the connected compartments. In addition, the area of the vent must be given and the shape is specified as either circular or square. Vents of other shapes must be replaced by equivalent[9] round or square openings. This is an example of a case in which the CFAST "vocabulary" restricts the user's ability to define the problem.

[8] The orientation of the vent is defined by the outward facing normal vector.

[9] In this context, "equivalent" refers to the flow resistance of the vent and not to the actual vent area. However, for vents that do not deviate too much from circular or square, adjusting the vent area is probably sufficient.

The CVENT keyword permits specification of horizontal vent closure events. The parameters for CVENT are the compartment numbers and the vent identification number (as defined by HVENT) and a list of fractional vent openings. The first fraction refers to the vent opening at zero time and subsequent entries correspond to successive event times, as established by FTIME. CVENT was included in the SHADWELL/688 simulations, but the vent width parameter was always set to 1.0 because, in the particular test selected for modeling, all of the vents were fully open during the fire. There is no corresponding keyword for vertical vents so, at present, it is not possible to define closure events for vertical vents.

The last keyword in this category is CFCON, which is used to enable vertical heat conduction through a ceiling/floor from the lower compartment to the upper. In the absence of this keyword, CFAST calculates outward heat conduction through the ceiling of the lower compartment, but does not include this energy as a heat source for the upper compartment. It is expected that it will be an important factor in most multi-deck, shipboard fire models due to the high conductivity of decks.

Horizontal heat conduction into adjoining compartments was not available at the time this work was performed but NIST has since added the HHEAT keyword to allow for this possibility. Validation of this new feature has not yet been performed, so the accuracy and utility of the horizontal conduction algorithm is not known.

2.1.5 Why specify the fire?

Before discussing the keywords used to define the fire, we address the obvious questions: Why do we need a fire specification at all? Why can we not simply specify the type and amount of fuel and allow the model to calculate the behavior of the fire as it develops?

This so-called self-consistent fire approach is possible in principle but is very difficult due to the nature of the chemistry involved. Fires involve an extremely complex set of interacting chemical reactions and any attempt to model them would require detailed information regarding the thermodynamics and kinetics of those reactions. More fundamentally, it would require the use of a field model, which would defeat the purposes of CFAST.

CFAST is a typical zone model in this respect because it makes no attempt to actually calculate the fire. In fact, it is somewhat misleading to refer to CFAST as a fire model: CFAST models the effects of the fire but does not actually model the fire itself. Rather than attempt to simulate chemical reactions, CFAST uses user-supplied species ratios to estimate the relative concentrations of various combustion products for a given quantity of burned fuel. The amount of fuel consumed is based on the user-specified fire size description.

The requirement for a specified fire is probably the most important restriction on the use of CFAST. As will be shown, there are a relatively large number of parameters involved in the fire specification and considerable effort must be expended to ensure that the description is internally consistent. Furthermore, if the goal of the model is to simulate a specific real fire (as was the case in this work), then additional work is required to verify that a match has been achieved.

For most "normal" fires (*i.e.*, those that do not involve explosions) the heat release rate of the fire is the most important single predictor of the hazard posed by the fire [11]. Therefore, we expect that the heat release rate will be the most critical input for prediction of temperature. If accurate predictions of oxygen or toxic gas concentrations are also needed, then a host of other parameters involving combustion chemistry factors will also be important.

Note that the fire specification discussed here applies to the so-called main fire, which ignites at time zero and then burns in accordance with the specification. In addition to the main fire,

CFAST provides a capability for specifying "object" fires which are intended to represent real objects, such as furniture, that may ignite during the course of the scenario. Depending on the user inputs, object fires ignite at a specified time, surface temperature or surface heat flux. Object fires were not used in our work and will not be discussed further.

2.1.6 Fire specification keywords

The most common fire specification keywords are given in Table A-4 and Listing 4 provides examples of their use. The location of the main fire is given by FPOS and LFBO. FPOS specifies the coordinates of the fire within the compartment, using the compartment coordinate system that was previously described. LFBO specifies the number of the compartment in which the fire is located.

```
#        X      Y      Z
FPOS    0.91   1.83   0.19
#Fire Cmpt
LFBO       1
#Fire Type (1 = unconstrained; 2 = constrained)
LFBT       2
#Mass pyrolysis rate
FMASS              0.0253    0.0229
#       Mol Wt    Rel Hum    LOL          Hc       Init T    Ign. T   Rad. fract.
CHEMI    184.       100.      10.    4.19E+007     285.9      330.       0.30
#H:C mass ratio (fuel composition)
HCR                0.143      0.143
#O:C mass ratio (fuel composition)
O2                 0.0        0.0
#HCN:fuel mass ratio (pyrolysis)
HCN                0.0        0.0
#HCl:fuel mass ratio (pyrolysis)
HCL                0.0        0.0
#Toxics:fuel mass ratio (pyrolysis)
CT                 0.0        0.0
#Soot:CO2 mass ratio (combustion)
OD                 0.06       0.06
#CO:CO2 mass ratio (combustion)
CO                 0.056      0.056
CJET OFF
```

Listing 4. Examples of the CFAST Fire Specification Keywords.

The fire is located, at the coordinates given in FPOS, in compartment one and is a constrained (type 2) fire. The fuel mass loss rate starts at 0.0253 kg/sec and declines to 0.0229 kg/sec at 1250 seconds. CHEMI specifies the fuel molecular weight and heat of combustion, as well as several other parameters. HCR and O2 specify the amount of hydrogen and oxidizing agent in the fuel, respectively; OD, CO, HCN, HCL and CT define the production rates for various pyrolysis and combustion products. CJET OFF invokes the standard ceiling jet convection algorithms.

Fires may be defined as either unconstrained (type one) or constrained (type two) by using the LFBT keyword. These types control the way in which the fire will respond to reductions in atmospheric oxygen concentration. In an unconstrained fire, CFAST always uses the specified heat release rate; for a constrained fire, the heat release rate will be reduced below the user-specified level if there is insufficient oxygen to support that combustion rate. We should also note that, for the unconstrained fire, CFAST does not calculate any species concentrations. The

assumption is that whenever there is enough oxygen to permit unconstrained burning the fuel will be completely oxidized to water and carbon dioxide.

The heat release rate of the fire is defined by the interaction of three different keywords: FQDOT, FMASS and CHEMI. The parameters associated with both FMASS and FQDOT are time-dependent — that is, they correspond to specific times defined by FTIME.

FMASS gives the pyrolysis (mass loss) rates of the fuel for the event times while FQDOT provides the actual heat release rates for those times. For each time, these values are related by

$$dQ/dt = \Delta H_c \, dm/dt \qquad \text{Eqn. 1}$$

where dQ/dt is the heat release rate (FQDOT), dm/dt is the mass loss rate (FMASS) and ΔH_c is the heat of combustion. The latter is one of the parameters included in the CHEMI line.

Obviously, if all three parameters are given, the fire is over-specified. CFAST only requires two of the three and, if all three are present, uses only the last two. For example, if a user includes the three keywords in the order FQDOT, FMASS and CHEMI, CFAST will use the FMASS values and ΔH_c to calculate new FQDOT values in accordance with Equation 1.

The CHEMI line is something of a catch-all. In addition to the heat of combustion, other parameters associated with this keyword are the molecular weight of the fuel, the initial relative humidity, the lower oxygen limit (LOL) of the fuel vapor, the initial fuel temperature, the fuel vapor ignition temperature and the radiative fraction. The significance of some of these parameters requires further explanation.

Natural concentrations of most atmospheric gases, such as oxygen, carbon dioxide and carbon monoxide, are relatively constant, regardless of location, season or weather conditions. However, water vapor concentration is highly variable so CFAST needs to be told what initial concentration to use. The relative humidity is used to calculate this initial value, which is then modified by the water contribution from combustion. Because water vapor is a strong absorber of infrared radiation, its concentration affects radiation transport and, therefore, temperatures. In addition, humidity is a factor in the calculation of hydrogen chloride deposition rates.

The lower oxygen limit (LOL) specifies an oxygen concentration (in volume percent) below which the fire will be extinguished. This limit is enforced only for the case of a type two (constrained) fire. The suppression function is very narrow, varying from one (no suppression) at LOL + 0.01 down to zero (extinguishment) at the LOL. The default value for LOL is 10%. This is a compromise, made by the CFAST developers, based on their observation that LOL is typically reported to be in the 15-17% range for small-scale fires but has been reported to approach zero in some large-scale fires [12]. Presumably, this discrepancy is related to turbulence, which could create oxygenated pockets in which combustion continues even when the nominal oxygen concentration is too low to support burning.

The energy generated by combustion can either heat the fire plume or, by radiation, heat the surrounding region. The ratio of radiated energy to total energy produced, the radiative fraction, is important because it strongly affects the relative temperatures of the gas layers, the walls, floor and ceiling. The default value is 30% and is appropriate for typical class B (fuel) fires. For very clean fires (methanol, for example), this value is probably too high.

There are seven other keywords, in addition to CHEMI, that affect the chemistry of the combustion process: HCR, O2, HCN, HCL, CT, OD and CO[10]. The first two of these are related to the fuel composition, the next three to the behavior of the fuel during pyrolysis and the last two to the combustion process. Collectively, these keywords provide the information used by CFAST to calculate the production of various pyrolysis and combustion products; the concentrations of these products are then tracked as they spread through the simulated system. The parameters associated with all of these keywords are treated as events so it is possible to specify fires in which the effective chemistry changes with time.

HCR and O2 are the hydrogen-to-carbon and oxygen-to-carbon mass ratios of the fuel, respectively. HCR is used to determine the amount of water vapor produced when the fuel is burned and O2 reflects the amount of oxidizer, if any, that is incorporated into the fuel. Any oxygen provided within the fuel itself reduces the need for atmospheric oxygen and therefore affects the heat release rate and oxygen consumption in constrained fires. The O2 keyword applies only to rocket fuels and other special cases. Fuels which contain oxygen within the molecular formula may be considered to be partially pre-oxidized (methanol can be thought of as partially oxidized methane, for example). In these cases, the effects of the oxygen are automatically accounted for by the heat of combustion and the O2 keyword is not needed.

HCN specifies the ratio of the mass of hydrogen cyanide in the pyrolyzate to the mass of pyrolyzed fuel. Similarly, HCL defines the mass ratio of hydrochloric acid to fuel. CT is similar to HCN and HCL in that it controls the rate of production of a pyrolysis product and this product is tracked as it spreads through the system. However, CT is not a real product, rather, it is a quantity which represents (based on empirical correlation functions) the total toxic hazard of the actual products. It takes into account the typical toxic effects of such things as carbon monoxide, acid gases and oxygen depletion. The CT input affects the predicted concentration of "total toxics" but does not affect the prediction of temperature or of any of the real fire products.

The last two keywords, OD and CO, specify mass ratios for products, but these ratios are calculated with respect to the mass of carbon dioxide in the product, rather than to the mass of the fuel. OD is the soot-to-carbon dioxide ratio and CO is the carbon monoxide-to-carbon dioxide ratio. OD strongly affects the predicted concentration of soot, of course, but also has a major indirect effect on temperatures because soot is usually the dominant term in calculating radiative energy transport.

The OD and CO ratios vary with combustion conditions and the user is responsible for providing physically reasonable values. This can be difficult for two reasons: (1) the parameters are ratios of products and any change in the combustion process that affects one product is likely to affect the other, making it difficult to intuitively estimate the net effect on the ratio; and (2) due to sensitivity to the combustion conditions, it is often not possible to find literature values appropriate to the simulation conditions. Furthermore, even if values consistent with the expected conditions are specified, the conditions calculated by the model may be very different from those expectations.

For example, suppose that you anticipate that the fire will always be well ventilated and specify an OD value that is appropriate for this case. If the model predicts some unanticipated ventilation effect (perhaps a vent closure far from the fire has a much greater effect than was anticipated), then the model may throttle back the fire (assuming it is a constrained fire). It is likely that the predicted soot production will then be too low (because CFAST will not increase soot production to account for the reduced oxygen) and, since temperatures are strongly affected by soot

[10] In common usage, OD refers to optical density while CO and O2 refer to the species carbon monoxide and oxygen, respectively. CFAST assigns different meanings to these terms and this non-standard usage sometimes causes confusion. In this report, OD, CO and O2 are always used in the CFAST sense and species are spelled out.

concentration, the model's temperature predictions may be grossly in error. The direct effect of the reduced heat release rate will be to lower temperatures in the vicinity of the fire, but the change in soot alters transport properties so that, further from the fire, temperatures could increase, decrease or remain the same.

It is important to understand that, except for HCR and O2, these parameters are not intrinsic to the fuel — they vary in response to changing combustion conditions. However, because CFAST does not calculate a self-consistent fire, it cannot account for this variation and will always calculate the composition of the pyrolysis products based on these user inputs.

CJET allows the user to select either the "standard" or the "ceiling jet" model of conductive heat transfer to the ceiling. During the initial stages of a fire, the fire plume rises rapidly and may "splash" against the ceiling, spreading radially from a point above the fire. This so-called ceiling jet can heat the ceiling more efficiently than the relatively quiescent gas layer that is more typical of later times. This effect can be important during the first few seconds of a fire, but normally becomes insignificant as the ceiling temperature approaches that of the gas and as the upper layer becomes thick enough to act as a buffer against the rising fire plume.

The value of the CJET parameter should be either "OFF" (ceiling jet convection algorithm disabled) or "CEILING" (jet convection enabled for the ceiling). In some earlier versions of CFAST, the values "WALL" and "ALL" were legal. "WALL" activated the jet algorithm for convection to walls; "ALL" enabled both ceiling and wall jets. However, it was found that the wall jet algorithm produced erroneous results and, consequently, that feature is no longer available in CFAST 3.1.4. The CJET parameter may still be set to "WALL" but the behavior of the model is the same as if "OFF" had been specified. Similarly, "ALL" produces the same effect as the "CEILING" parameter.

There are two additional fire specification keywords that should be mentioned, although they were not used in this work. FHIGH specifies the height of the base of the flames above the position specified by FPOS. FPOS is a constant but FHIGH is treated as an event, so this keyword provides a mechanism for varying the elevation of the fire with time. For example, it could be used to simulate a debris pile in which the base of the fire decreases as the pile burns down. Since our simulations used pool fires in which the depth of the pan was negligible relative to the height of the compartment, this keyword was not needed.

FAREA specifies the horizontal area of the base of the flame. It was provided so that sophisticated plume models, in which entrainment is a function of fire area, could be incorporated into CFAST. However, those plume models were never added to CFAST and, at present, FAREA is not used.

3.0 DEVELOPMENT OF A FIRE SPECIFICATION

In this section, we discuss the development of a fire specification for the particular case of Submarine Ventilation Doctrine test 4_10. This process was similar to that which we would expect to be followed in applying CFAST to a hypothetical new ship design, except for one factor: in order to compare our results with the test data, we had to simulate a specific fire. In contrast, the ship designer has no *a priori* target fire. Instead, we anticipate that a variety of fires, representing many possible casualties, would be simulated during the design process.

3.1 Defining the Laundry Room Model

Although the goal of this section is to provide guidance for development of the fire specification, it is important to realize that CFAST cannot run with only a fire specification. Before the model can be run, we must define all of the non-fire parameters, discussed in the previous section, for

the fire compartment. For this case study, the fire compartment was the Laundry Room, which is illustrated in Figure 3. The simplicity of this compartment minimizes the difficulties in setting up those parameters and, in fact, that was one of the reasons for selecting test 4_10 as the subject for this case study. The CFAST input file describing this single-compartment simulation is shown in Listing 5.

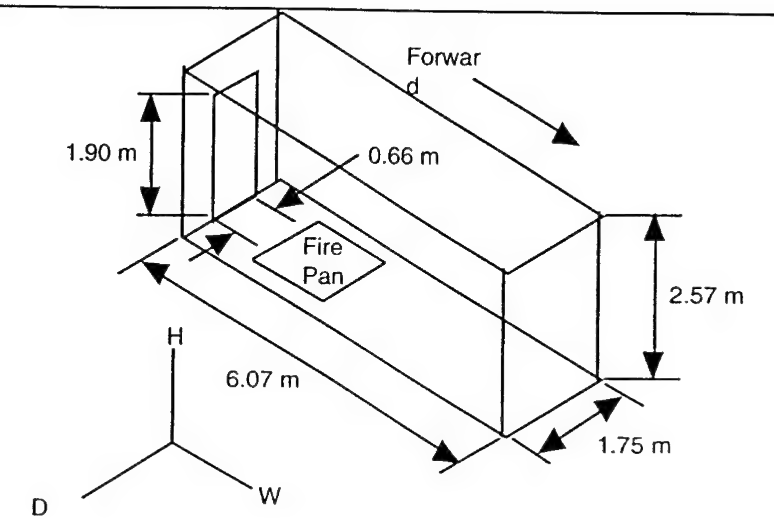

Figure 3. Laundry Room Dimensions

```
VERSN     3 SHADWELL/688 Laundry compartment
#        Sim.time  Print  Hist.  Disp.  Copies
TIMES      1250      1      3      0      0
#                  t0      t1
FTIME                     1250.
DUMPR model.HI
#          Temp.    Press.     Elev.
TAMB     285.900   101300.   0.000000
EAMB     286.300   101300.   0.000000
#        Cmpt. 1
#        Laundry
#Floor elevation
HI/F     0.00
#X dimen.
DEPTH    1.75
#Y dimen.
WIDTH    6.07
#Z dimen.
HEIGH    2.57
#Materials
CEILI    SHIP3/8
WALLS    SHIPLR
FLOOR    SHIP3/8
```

Listing 5. CFAST Input File for the Laundry Room Simulation

This simple, one-compartment model of the Laundry Room was used for development of the fire specification.

```
#       Cmpt#    Cmpt#    Vent#    Width     Soffit     Sill
HVENT   1        2        1        0.66      1.90       0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0  Width@t1
CVENT   1        2        1        1.00000   1.00000
#Fire Cmpt
LFBO        1
#         X       Y       Z
FPOS    0.91    1.83    0.19
#Fire Type (1 = unconstrained; 2 = constrained)
LFBT        2
#Mass pyrolysis rate
FMASS              0.0253    0.0229
#        Mol Wt    Rel Hum    LOL        Hc         Init T    Ign. T    Rad. fract.
CHEMI     184.       100.     10.    4.19E+007     285.9      330.        0.30
#H:C mass ratio (fuel composition)
HCR                0.143      0.143
#O:C mass ratio (fuel composition)
O2                 0.0        0.0
#HCN:fuel mass ratio (pyrolysis)
HCN                0.0        0.0
#HCl:fuel mass ratio (pyrolysis)
HCL                0.0        0.0
#Toxics:fuel mass ratio (pyrolysis)
CT                 0.0        0.0
#Soot:CO2 mass ratio (combustion)
OD                 0.06       0.06
#CO:CO2 mass ratio (combustion)
CO                 0.056      0.056
CJET OFF
```

Listing 5 (cont'd). CFAST Input File for the Laundry Room Simulation

3.1.1 Simulation control

For these simulations, the only important control parameters were the simulation time (TIMES) and the event schedule (FTIME). The actual test lasted approximately 1320 seconds, but the fire began to die somewhat before that so the simulation time was set to 1250 seconds. The only time-related factor that directly affected the fire was the slow change in mass loss rate during the test. As is discussed below, this change was nearly linear, so it was sufficient to specify mass loss rates only for the start and end of the test. Accordingly, FTIME defines a single event time at 1250 seconds (recall that there is an implicit event time at zero seconds). The output file (DUMPR) was given a generic name, MODEL.HI, and no restart file was needed since these simulation began at time zero.

3.1.2 Ambient environment

Since our immediate goal was to model the conditions of one specific fire, we used actual pre-ignition air temperatures for the compartment and external ambient temperatures. Typically, shipboard temperatures do not vary widely from compartment to compartment so, in the absence of specific temperature information, it would be reasonable to use 298 K (25 °C) for normal living spaces. For special cases, such as machinery space fires, it might be necessary to use higher values, depending on whether the simulation applies to a steam, gas turbine or nuclear ship. In any case, the effects of different ambient temperatures are not likely to be very significant.

For the test case, ambient temperatures were determined by taking the average of all air temperature readings during the period prior to ignition. The values for the Laundry Room

(285.9 K) and the Laundry Passageway (286.3 K) were used for the initial temperature parameters for TAMB and EAMB, respectively. The rationale for using the passageway, rather than the exterior, temperature for EAMB was that, from the perspective of the fire compartment, the passageway is the exterior. That is, air entering through the door will be at passageway temperature and conduction through the walls will be governed by the temperature difference between the laundry and the passageway.

Of course, conduction through the deck and overhead areas involves other compartments, which may be at different temperatures. Most of the test area was at about the same temperature (within several degrees), so this is not likely to introduce a significant error. In any case, the limitation of being able to specify only a single "external" temperature makes this type of approximation unavoidable.

Pressures for both TAMB and EAMB were set to 101300 Pa (one atmosphere) and the reference elevations were set to zero (sea level). As was mentioned previously, the absolute elevation is significant only when modeling high-rise buildings. For a model in which the maximum elevation differences are only on the order of a few tens of meters, these parameters are not important.

3.1.3 Laundry Room geometry

The Laundry Room deck elevation was set to zero (HI/F), which implies that the TAMB and EAMB reference points are at this level. Since this compartment is a rectangular parallelepiped, we can immediately specify the DEPTH, WIDTH and HEIGH parameters as 1.75 m (5.74 ft), 6.07 m (19.9 ft), and 2.57 m (8.43 ft), respectively. Note that we have adopted the convention that width (y-axis) is parallel to the length of the ship and that depth (x-axis) is in the athwartship direction. Because this compartment meets the CFAST constraint that all surfaces are assumed to be rectangles, we are able to represent the geometry exactly, with no approximations.

All of the boundaries of the Laundry Room were constructed of steel of various thickness. Since the SHADWELL/688 test area was heavily sooted, the entries for steel in the thermal properties database, THERMAL.DF, were edited to change the emissivity from the default value (0.9), which is typical of clean steel, to 1.0, which is a reasonable value for steel coated with carbon black.

The Laundry Room overhead (CEILI) and deck (FLOOR) were constructed of 0.95 cm (0.38 in.) steel, which is one of the values (SHIP3/8) in THERMAL.DF. However, the bulkheads (WALLS) were made of several steel plates, of different thicknesses, welded together. Since CFAST does not permit the use of multiple materials for any single boundary, we defined a fictitious material, SHIPLR, to represent these bulkheads. Because the plates were made of the same material, we used the standard thermophysical properties (density, conductivity and heat capacity, for example) of steel and varied only the thickness. To ensure that the effective heat capacity of the model bulkhead was the same as the total of the actual bulkheads, we required that our bulkhead mass equal to the actual mass. This implied that the material volumes would also be equal and it followed that the area-weighted mean was the proper average to use for the thickness. Based on this, SHIPLR was specified to have a thickness of 0.0076 m (0.30 in.). The relevant portions of the modified version of THERMAL.DF are shown in Table 2.

The joiner door leading into the Laundry Passageway was defined as an HVENT connecting compartment one (Laundry Room) to compartment two (the exterior of the modeling domain). This was vent number one and had a width of 0.66 m (2.2 ft), a soffit of 1.90 m (6.23 ft) and a sill at zero. The vent was always fully open, so the parameters of the corresponding CVENT were set to 1.0 for both event times.

Material	Conductivity (W/m/K)	Specific Heat (J/kg/K)	Density (kg/m^3)	Thickness (m)	Emissivity
SHIP2/8	48	559	7854	0.0064	1
SHIP3/8	48	559	7854	0.0095	1
SHIP4/8	48	559	7854	0.0127	1
SHIP5/8	48	559	7854	0.0159	1
SHIPLR	48	559	7854	0.0076	1

Table 2. Material Property Database Entries for Steel Plate.

The material properties database (THERMAL.DF) used for the Laundry Room simulations contains several entries for the various thicknesses of steel plate used in the SHADWELL test area. The SHIPLR entry was created specifically for this simulation; the other entries are standard thicknesses of steel. Emissivities were set to one (rather than the default 0.9) because surfaces in the test area were covered with soot.

3.2 The Fire Specification

The fire was located in compartment one, as defined by LFBO, with the pan centered at 0.91 m (D) x 1.83 m (W) (2.99 ft x 6.00 ft) relative to the compartment origin. The load cell, used for mass loss measurements, elevated the pan 0.19 m above the deck. These coordinates were given with the FPOS keyword and LFBT specified a constrained (type two) fire so that the effects of oxygen depletion would be included in the calculations. The area of the fire, 0.87 m^2 (9.37 ft^2) was not included because the current version of CFAST does not use this information (recall the previous discussion of the FAREA keyword).

In CFAST, burning is treated as a two-step process,

$$\text{Fuel} \rightarrow \text{Fuel vapor} + \text{Pyrolysis products} \qquad \text{Eqn. 2a}$$

$$\text{Fuel vapor} + \text{Oxygen} \rightarrow \text{Combustion products} \qquad \text{Eqn. 2b}$$

where Equations 2a and 2b represent pyrolysis and combustion, respectively.

Many of the fire specification parameters may be categorized as fuel, pyrolysis or combustion parameters, depending on which part of the overall process they affect. These three classes of parameters are considered in the following three sections.

3.2.1 Fuel parameters

Fuel parameters are often the easiest to specify because they depend only on the nature of the fuel and are independent of the details of the burning process. Offsetting this is the fact that the properties of most real fuels (as opposed to those of chemically pure surrogates, such as hexane) have high batch-to-batch variability and few batches are characterized in any significant way. Values for many fuels may often be obtained from the literature, including chemical handbooks, military and standards organization specifications[11] and similar references. It is important to keep in mind that many of these sources, especially standards documents, only provide upper or lower

[11] The American Society for Testing and Materials (ASTM) is one example of such a standards organization.

limits. As a result, literature values must be considered to be estimates, rather than exact values, for the properties of any given fuel batch.

Fortunately, this problem is usually not critically important because, in most cases, we have no way of knowing the details of some hypothetical future fire and therefore must consider a range of possibilities. It is reasonable to start with nominal values taken from these references, on the assumption that they will be representative of typical batches of the given fuel. Simulations should then be run using a range of deviations from the nominal values to account for the possibility that some fuels will be atypical — out of specification or contaminated with other fuels, for example.

In our case, the fuel was a marine diesel, but no further details were given. We used values taken from Table 5.2 of Kanury [13] for the molecular weight (184 gm/mol) and for the heat of combustion [4.19×10^7 J/Kg (1.80×10^4 BTU/lb)]. The vapor ignition temperature was estimated from the minimum flash point for number two diesel fuel, which is given as 52 °C in the ASTM specification for diesel fuels [14]. Since all refiners provide a safety margin above this minimum requirement, we assumed that the actual ignition temperature would be 10% higher, or 57 °C (330 K). All three of these are specified as parameters of the CHEMI keyword.

According to the fuel specification [15], the minimum hydrogen content of F-76 diesel fuel is 12.5% by weight. Using this value, and the molecular weight of the fuel, we estimated HCR to be 0.143. We ran simulations with a range of HCR values, as discussed in detail in reference [6], and found that this parameter had only a limited impact on the model predictions in most cases. These fuel characteristics, and the sources for the values, are summarized in Table 3. Finally, since the fuel used in the SHADWELL/688 tests had no included oxidizing agent, the oxygen-carbon ratio (O2) was zero.

Property	Value	Source
Molecular Weight (gm/mol)	184	[11]
Heat of Combustion (J/Kg)	4.19 x 10^7	[11]
Ignition Temperature (K)	330	[12]
Min. Hydrogen Fraction (%)	12.5	[13]

Table 3. Typical Properties for Marine Diesel Fuel.

3.2.2 Pyrolysis parameters

The pyrolysis process, illustrated in Equation 2a, involves evaporation or thermal decomposition of the (assumed) solid or liquid fuel[12]. During this process, some fuel components evaporate to form a fuel vapor, others may break apart into lower molecular weight species which then evaporate as more fuel vapor (this is typical of some plastics and other polymers) and still others decompose directly to form products without undergoing combustion. The latter mechanism typifies the production of acid gases, such as hydrochloric acid and hydrogen cyanide.

Because the goal of this work was to determine how well CFAST simulated a specific test fire, it was very important that the fire description accurately represent the actual fire. Therefore, the pyrolysis rate (FMASS) inputs were calculated from actual test data. To reduce the experimental

[12] Some fuels (methanol, for example) evaporate to form a flammable vapor; other (such as plastics) undergo a chemical decomposition (pyrolysis) process first so that the vapor is chemically dissimilar to the original fuel. CFAST does not distinguish between these two cases — FMASS represents the total mass lost from the original fuel, without regard to whether thermal degradation was involved.

noise, the fuel mass data were smoothed (five-point sliding average) and plotted as a function of time, as shown in Figure 4. We found that the data could be closely fitted with the exponential curve shown in the figure ($R^2 = 0.955$), which was then used to calculate the mass loss rate curve. The latter was very nearly linear ($R^2 > 0.9998$), and, since CFAST uses linear interpolation between event times, FMASS was defined by the mass loss rates at zero and 1250 seconds [0.0253 and 0.0229 kg/s (0.0558 and 0.0505 lb/s), respectively].

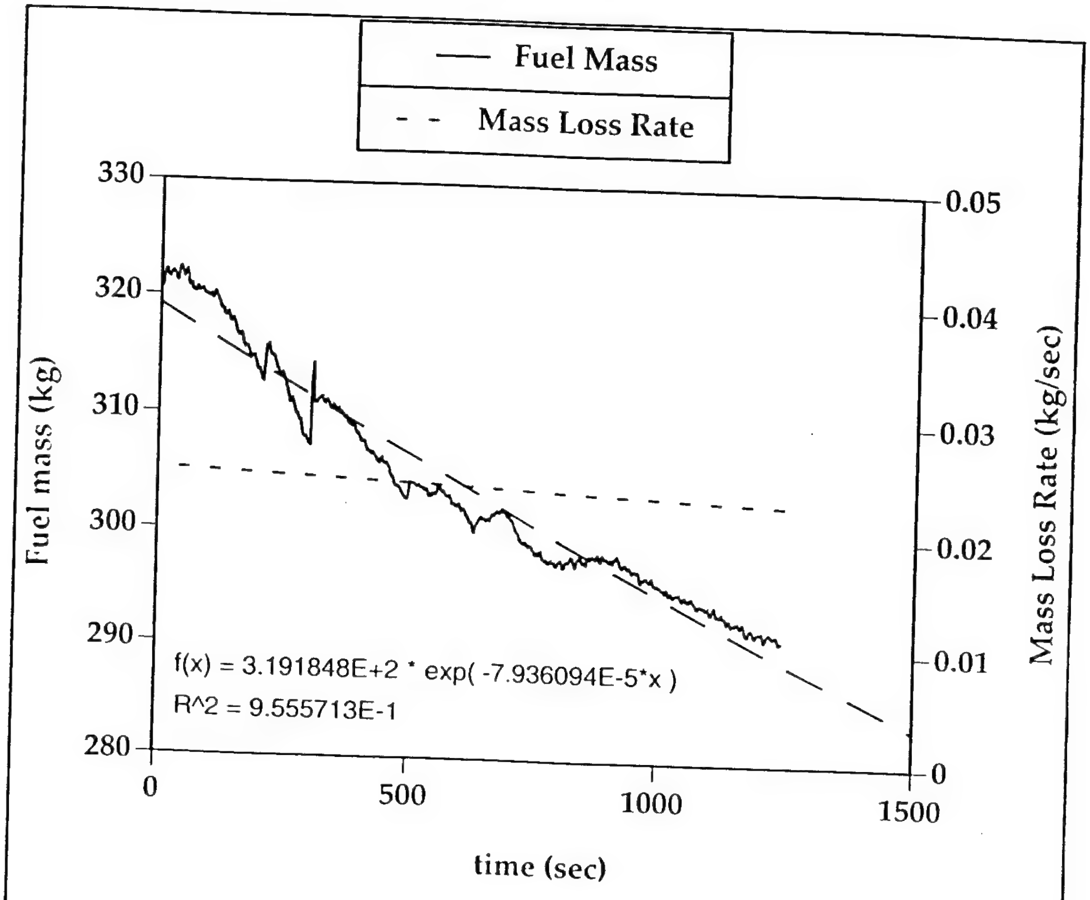

Figure 4. Fuel Mass and Mass Loss Rate

There are three CFAST parameters that are related to the fuel decomposition process: HCN, HCL and CT. These are, respectively, the mass ratios for hydrogen cyanide-fuel, hydrogen chloride-fuel and total toxics-fuel. Recall that "total toxics" is a fictitious species that attempts to summarize the overall toxicity of the combustion products. Note that, unlike the HCR and O2 parameters, which were defined in terms of the mass of carbon in the fuel, the pyrolysis parameters are referenced to the total fuel mass.

Since we assumed that the our fuel was a pure hydrocarbon, there were no nitrogen- or chlorine-containing compounds in the fuel. This allowed us to set the HCN and HCL parameters to zero. Further, we were not interested in trying to represent toxicity as a single number, preferring to separately consider each of the possible toxic species. Consequently, we also set CT equal to zero.

If it were known, or suspected, that the fuel contained significant amounts of nitrogen or chlorine (for example, if it had been a polyvinylchloride cable insulation), it would have been necessary to find appropriate, non-zero values for these inputs. Frequently, materials specifications include

either maximum or minimum allowable concentrations (sometimes both) for contaminant species (*e.g.*, nitrogen compounds in fuels); in those cases, it would be reasonable to estimate values for HCN and HCL following a procedure similar to that used for HCR.

3.2.3 Combustion parameters

The combustion process, shown in Equation 2b, is usually the most difficult to handle because the parameters involved are a function of the combustion conditions, which we do not know *a priori*. The primary parameters in this category are the production factors for soot and for carbon monoxide (OD and CO, respectively).

CFAST calculates the reduction in combustion due to oxygen depletion[13] but does not account for the changes in the combustion product ratios that also occur when the fire is oxygen starved. Thus, we are in the position of trying to guess what the burning conditions will be so that we can provide the correct product ratio inputs, when those very inputs influence the burning conditions. As previously mentioned, the inability of CFAST to dynamically adjust the combustion parameters as a function of instantaneous conditions is probably the most significant shortcoming of the model. Unfortunately, accurate combustion calculations would require the use of a field model incorporating detailed reaction kinetics and that would negate the advantages of a fast, simple zone model.

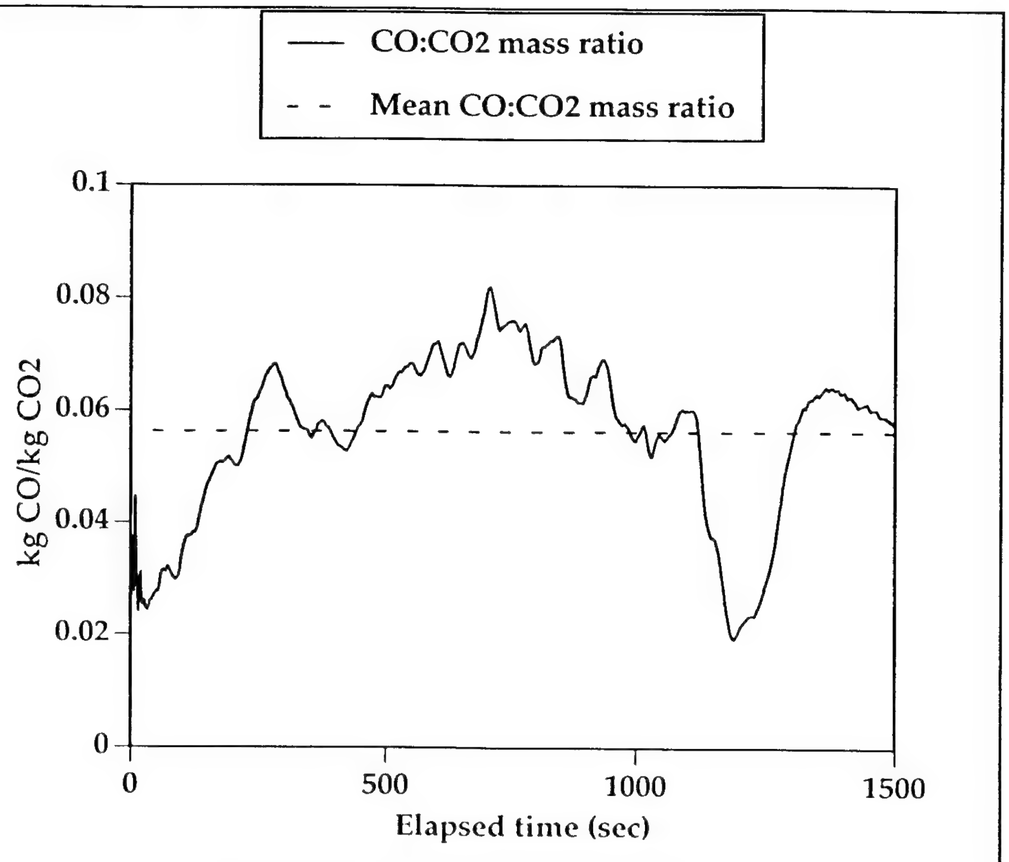

Figure 5. Experimental $CO:CO_2$ Ratio

[13] This assumes that a constrained fire has been specified, as was the case in our work.

For our Laundry Room model, we tried several values for OD, ranging from zero to 0.10. Temperatures were found to be highly dependent on the presence or absence of soot but relatively insensitive to the exact value of OD for values greater than about 0.04. Ultimately, we chose 0.06 as an appropriate estimate for diesel fires. For fuels that are expected to burn cleanly (methanol, for example), it would be important to use a value near zero.

Carbon monoxide production is extremely variable from fire to fire and the literature is of little help to us. For flaming fires, the maximum mass ratio of carbon monoxide to carbon dioxide is expected to be about 0.013 [16]. The CFAST default value, 0.05, is probably a reasonable mean value for a "typical" fire which would include non-flaming periods. Based on test data (Figure 5), we determined that a CO parameter value of 0.056 was reasonable for test 4_10.

Fortunately, the CO input had little effect on temperature predictions so, in many cases, this parameter is not critical to the fire specification and it may be acceptable to use an arbitrary value near 0.05. However, if the carbon monoxide concentrations are important, then the CO parameter does become critical. Without a correct value for this parameter, concentration predictions will be very inaccurate. At present, there does not appear to be a good solution to this problem. The best approach is probably to run the simulation with a variety of different CO inputs and present the results as a range of possible concentrations.

3.2.4 Miscellaneous parameters

There are several additional parameters which affect the fire or species calculations but do not fall into any of the above categories. These include the initial fuel temperature, the relative humidity, the lower oxygen limit, the radiative fraction and the CJET setting.

For our simulations, the initial fuel temperature was set to the laundry room ambient temperature, on the assumption that the fuel pans were approximately in thermal equilibrium with the compartment prior to ignition of the fuel.

Due to the large amounts of water liberated by the repeated fire tests, it was reasonable to assume that the atmosphere would be saturated. Therefore, a relative humidity value of 100% was used.

Default values for the lower oxygen limit (LOL) and radiative fraction inputs (30% and 10%, respectively) were used because those were believed to be reasonable values for diesel fuels and no better information was available. The radiation fraction is dependent on the amount of soot in the fire plume and, in real fires, that is controlled partly by the nature of the fuel (for example, saturated fuels typically produce cleaner fires than do highly unsaturated fuels) and partly by the amount of available oxygen.

With CFAST, the amount of soot is controlled by the OD input, as previously discussed, and the radiative fraction should be consistent with OD. The defaults for these parameters are appropriate for "dirty" fuels but, for "clean" fuels (such a methanol), both the radiative fraction and OD should be reduced.

As discussed previously, the ceiling jet algorithm affects only the first few seconds of the simulation. Since we were interested primarily in the model predictions for long time periods (tens of minutes), we set CJET to "OFF" for this work.

3.3 Results of the Fire Specification Development

The Laundry Room was modeled (using the fire specification described above) and the model predictions were compared with thermocouple data from the test. That comparison is presented

in this section. Our primary purpose here is to illustrate the general performance that may be obtained from the CFAST model.

However, prior to making this comparison, it was necessary to determine which thermocouples measured the upper layer and which the lower layer. In the following paragraphs we briefly discuss the experimental data processing methodology and explain how the thermocouples were apportioned between the layers.

The Laundry Room was instrumented with a single thermocouple tree, illustrated in Figure 6, that had thermocouples at elevations of 0.14 m (0.46 ft), 0.50 m (1.64 ft), 0.95 m (3.12 ft), 1.27 m (4.17 ft), 1.94 m (6.37 ft) and 2.50 m (8.20 ft) above the deck. The temperature reported by each thermocouple was recorded at one second intervals for several minutes prior to ignition of the test fire and the Laundry Room pre-ignition temperature was calculated as the ensemble average (the mean of all measurements for all thermocouples). Zero point offset errors were corrected by adjusting the readings so that the mean pre-ignition temperatures for each thermocouple was equal to the ensemble mean.

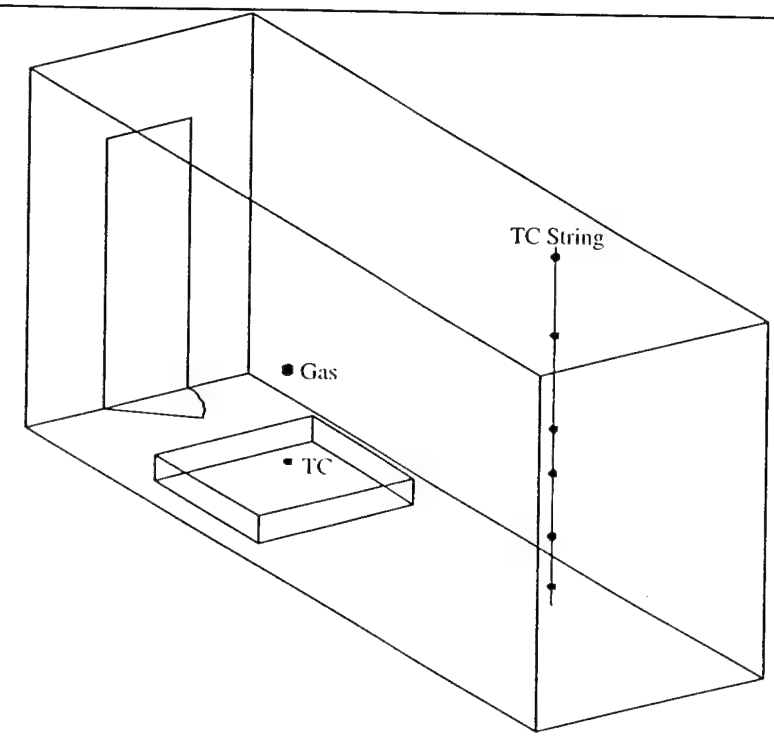

Figure 6. Locations of Laundry Room Thermocouples

The CFAST-predicted interface height (Figure 7) was then used as the demarcation between lower and upper layer thermocouples. Ignoring the transients that occurred during the first several seconds, the interface was found to lie at approximately 0.6 m. Accordingly, the bottom two thermocouples were assigned to the lower layer and the top four to the upper layer.

For each layer, the appropriate thermocouples were averaged and the population standard deviation was estimated. As seen in Figure 8A (upper layer) and Figure 8B (lower layer), the predicted temperatures were very close to the measured values (well within one standard deviation) except at the start of the fire. During that early period, CFAST consistently overestimated the air temperatures.

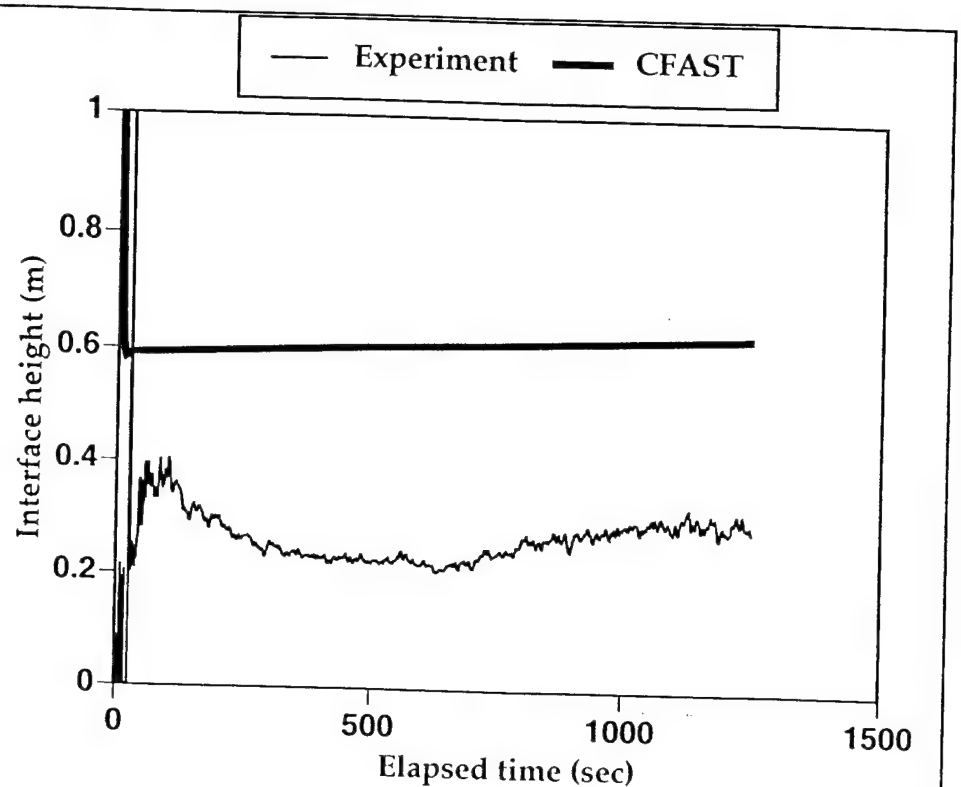

Figure 7. Laundry Room Interface Height

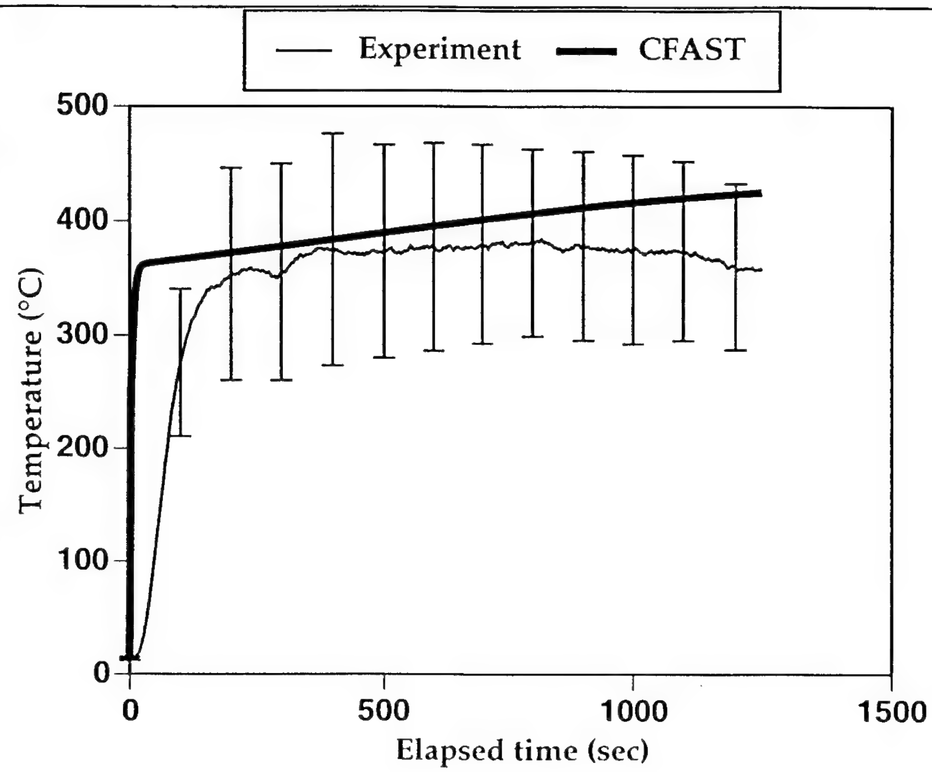

Figure 8A. Comparison of Actual and Predicted Upper Layer Temperatures for the Laundry Room

The error bars represent one standard deviation in the test data. The assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

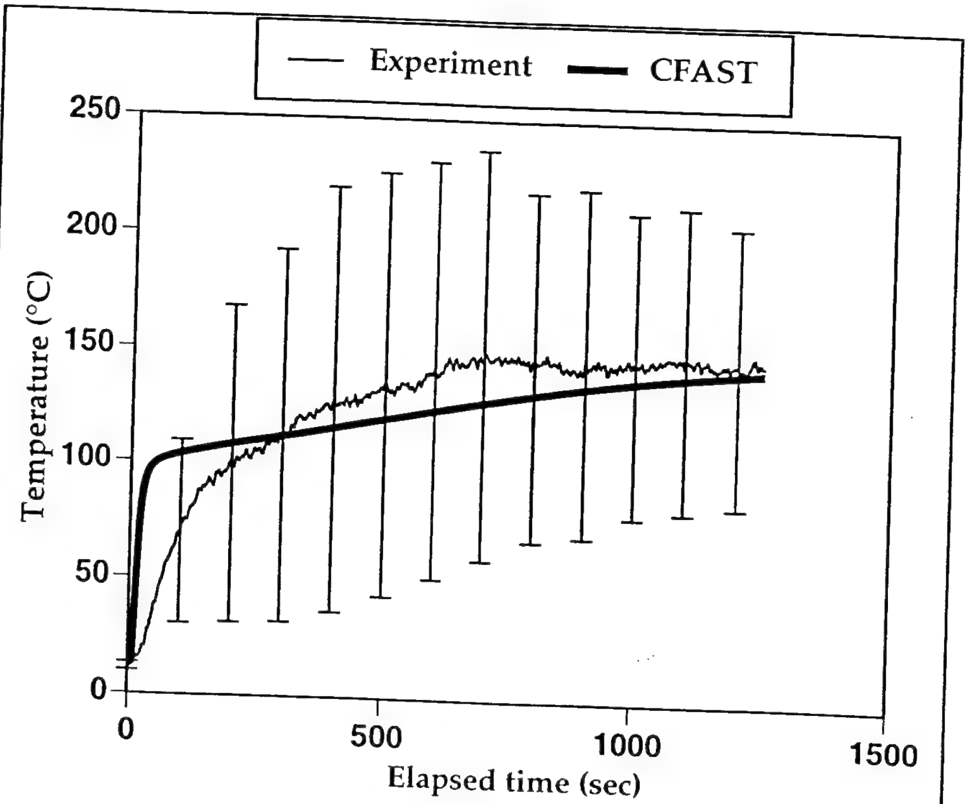

Figure 8B. Comparison of Actual and Predicted Lower Layer Temperatures for the Laundry Room

The error bars represent one standard deviation in the test data. The assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

4.0 DEVELOPMENT OF A GEOMETRY SPECIFICATION

The geometry of the Laundry Room was sufficiently simple that no approximations were needed, except for the correction to the bulkhead thickness. However, most of the other compartments required significant simplification before the geometry could be specified in a manner compatible with CFAST limitations.

We will consider three classes of problems which were found to be significant: 1) non-rectangular geometry, 2) vertical transport and 3) ambiguous thermophysical properties. The Laundry Passageway provided the best example of the difficulties in dealing with non-rectangular geometry and also provided an example of mass transport through a vertical vent. The Wardroom added vertical conduction to the model and, in the Navigation Equipment Room, we encountered a case in which the standard thermophysical properties were not applicable. In this section, we illustrate the approximation techniques used and present the rationales for each. The details of the modeling of these compartments have been reported previously [7] and will not be repeated here.

4.1 Problems of Non-Rectangular Geometry

As may be readily seen from Figure 9, the deck plan of this compartment is approximately L-shaped. In addition, the compartment tapers from fore to aft and the lower portion of the

outboard bulkhead is cut away, producing a five-sided vertical cross section. Any one of these factors would make it impossible to create an exact description for CFAST. In addition, the bulkheads were made of several different thickness of steel plate.

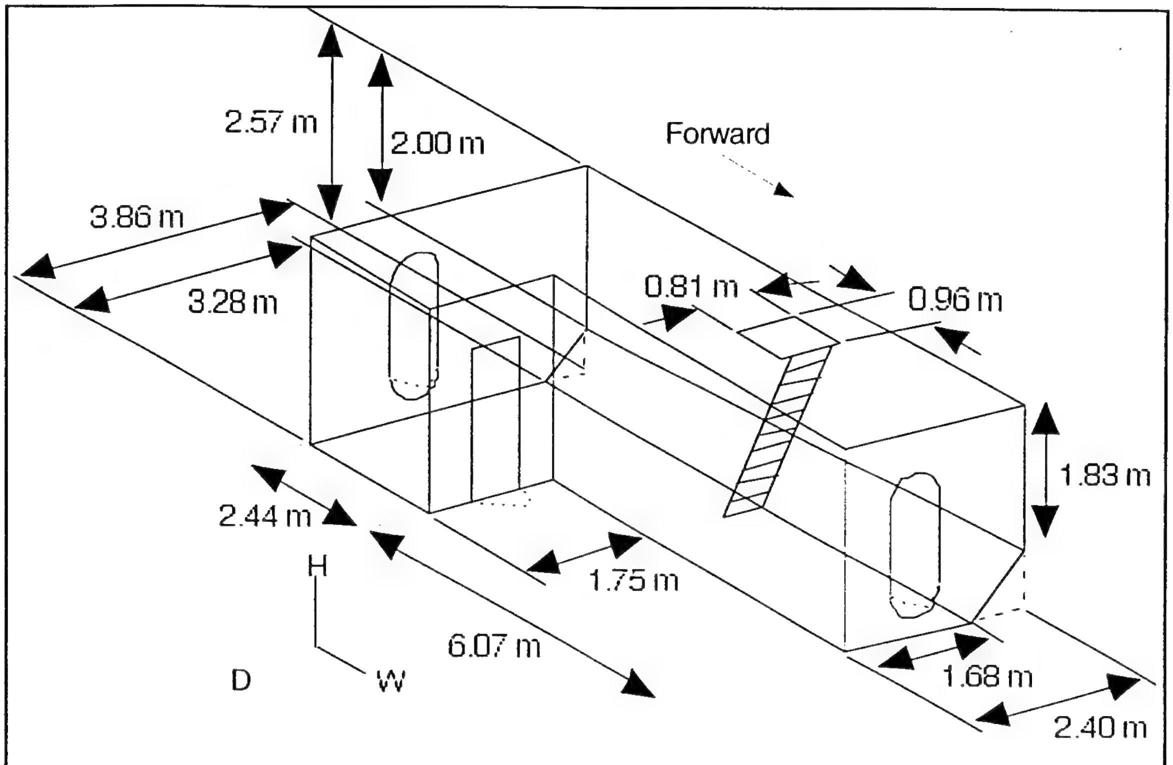

Figure 9. Laundry Passageway Dimensions

There were three horizontal vents and one vertical vent in the Laundry Passageway. One of the horizontal vents was already included in the model as part of the Laundry Room; the other two were standard Navy water tight hatches having a 0.66 m (2.17 ft) width, a 0.23 m (0.75 ft) sill and a 2.04 m (6.69 ft) soffit. Unlike the Laundry Room door, these hatches had rounded corners, but the radius of curvature was negligible (on the order of a few centimeters). All of these vents were fully opened during the tests, so each of the fractional openings (defined by the CVENT parameters) was set to 1.0. The new vents were defined as connecting compartments two (Laundry Room) and three (exterior). For consistency with the Laundry Room, the deck elevation was set to zero.

In this section, we present some approaches to approximating compartment dimensions. Issues related to vertical transport and thermophysical properties will be addressed in subsequent sections. However, before considering the details of our methods, we will discuss some considerations that may be more broadly applicable.

4.1.1 General considerations

We previously noted that CFAST was designed with the assumptions that each compartment has exactly six bounding surface and that each surface is rectangular. These assumptions are implicit in the equations used to calculate surface areas.

$$A_{deck} = A_{ovhd} = \text{DEPTH} * \text{WIDTH} \qquad \text{Eqn. 3a}$$

$$A_{\text{lower blkhd}} = 2 * (\text{DEPTH} + \text{WIDTH}) * \text{I} \qquad \text{Eqn. 3b}$$

$$A_{\text{upper blkhd}} = 2 * (\text{DEPTH} + \text{WIDTH}) * (\text{HEIGH} - \text{I}) \qquad \text{Eqn. 3c}$$

where I is the height of the interface between the lower and upper zones, measured from the deck of the compartment.

Likewise the equations for the zone volumes are

$$V_{\text{lower}} = \text{DEPTH} * \text{WIDTH} * \text{I} \qquad \text{Eqn. 4a}$$

$$V_{\text{upper}} = \text{DEPTH} * \text{WIDTH} * (\text{HEIGH} - \text{I}) \qquad \text{Eqn. 4b}$$

As long as the compartment is a rectangular parallelepiped, Equations 3 and 4 are correct and self-consistent. However, a problem arises if the compartment is not a rectangular parallelepiped. In that case, three dimension parameters are not sufficient for an accurate description. The three inputs can be adjusted so that some of these equations are correct, but there is no combination of inputs that can make all of them simultaneously correct. So, how do we decide which equations to satisfy and which to sacrifice?

First, consider the fire compartment. Conditions there are largely determined by the fire specification, which defines the production rates for mass and energy, and by the compartment volume. The latter dictates how much dilution occurs and, therefore, affects the concentrations and temperatures. For the other compartments, mass and energy transport play important roles. Transport equations include a driving force term (pressure, temperature or concentration, for example) and a resistance term. Typically, these terms are inversely proportional to volume and area, respectively. Thus, the transport equations have both volume and area dependencies.

Based on the above considerations, we expect that zone volumes will affect both the conditions in the zone and the mass and energy transport between zones. Since volume has significant effects on every aspect of the fire model, we considered it to be the most critical factor. Accordingly, we imposed the requirement that our approximate compartment dimensions be chosen so as to give the correct volumes. Surface areas were deemed to be of less importance because they directly influence only the transport equations.

Another consideration involves transport through horizontal vents. For each of the connected compartments, a horizontal vent may be located in the lower layer, the upper layer or it may span both layers[14]. Since the layer interface is dynamic, transport through a horizontal vent can be very complex and is clearly a function of the interface height, as well as of the vent parameters.

The interface starts at the top of the compartment and grows downward as the volume of gas in the upper layer increases. Consequently, the difference in elevation between the overhead and the vent soffit is an important factor in determining horizontal vent flow. In order to make these flows as accurate as possible, we endeavored to use the correct compartment heights at the expense of compartment depths and widths.

[14] Note that vertical vents do not have this degree of complexity. Because they always reside at the interface between the upper layer of one compartment and the lower layer of another, they can never span layers.

Unfortunately, given the constraint of a fixed volume, surface areas and compartment heights are not independent parameters. By fixing volume and height , we have implicitly fixed the overhead and deck areas as

$$A_{deck} = A_{ovhd} = V_{act} / H_{act} = DEPTH * WIDTH \qquad \text{Eqn. 5}$$

where V_{act} and H_{act} are the actual volume and height of the compartment. The only remaining option is to specify either DEPTH or WIDTH, the other being determined by Equation 5.

This approach works well if our primary interest is in horizontal fire spread and there are horizontal vents. However, if the primary goal is to simulate vertical conduction through decks, then it is important that the overhead and deck areas be accurate. In that case, a better procedure might be to conserve compartment volumes and overhead areas. The compartment height would then be

$$HEIGH = V_{act} / A_{act\ ovhd} \qquad \text{Eqn. 6}$$

where $A_{act\ ovhd}$ is the actual area of the compartment overhead. This again provides some freedom in selecting DEPTH or WIDTH but we must realize that horizontal vent flows will be less accurate with this approach.

In either case, the choice of DEPTH and WIDTH is somewhat arbitrary. In our work, we used the actual value of one of these parameters, if an unambiguous value was available. Since the version of CFAST available for this project does not support horizontal heat conduction between compartments, we did not make a special effort to correctly specify bulkhead areas. We did, however, compare the actual and approximated surface areas in order to estimate the amount of error introduced into the model.

Because vents directly influence both mass and energy transport, correctly specifying the vent parameters was also important. Vent areas and shapes were chosen to be as accurate as possible. In our simulations, vertical vents always required some approximation since the hatches were rectangular rather than square.

4.1.2 Estimation of actual volumes

In determining the Laundry Passageway dimensions, our first step was to estimate, as accurately as possible, the actual volume of the compartment. Due to the complexity of the Laundry Passageway, this process was somewhat complicated.

As shown in Figure 10, the Laundry Passageway was divided into two parts, Section 1 and Section 2, such that the actual compartment volume was conserved

$$V = V_1 + V_2 \qquad \text{Eqn. 7}$$

where V is the total Laundry Passageway volume and V_1 and V_2 are the volumes of Section 1 and Section 2, respectively.

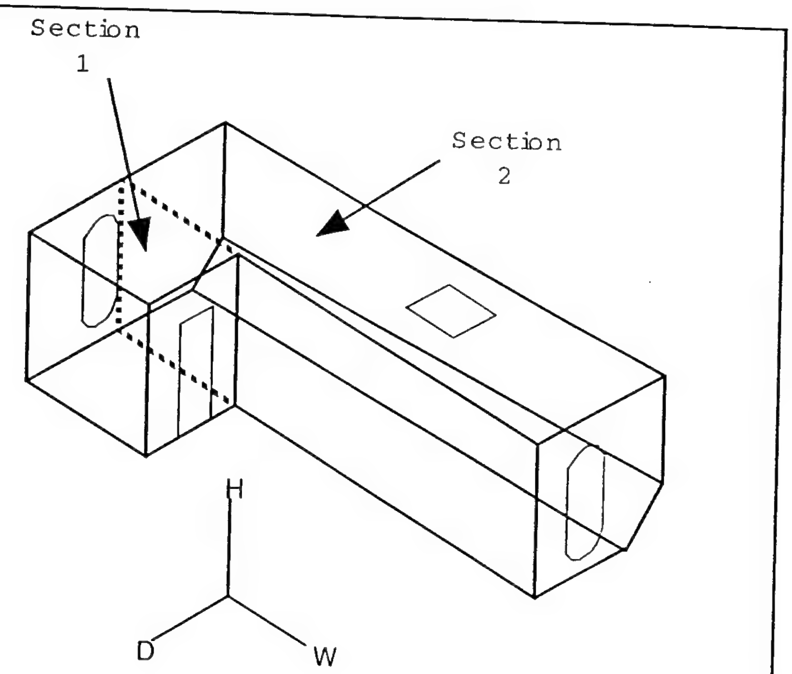

Figure 10. Conceptual Division of the Laundry Room Passageway into Sections

For Section 1, the volume is

$$V_1 = H_1 * W_1 * D_1 \qquad \text{Eqn. 8}$$

and the dimensions may be read directly from Figure 9

$$H_1 = 2.57 \text{ m} \qquad \text{Eqn. 9a}$$

$$W_1 = 2.44 \text{ m} \qquad \text{Eqn. 9b}$$

$$D_1 = 1.75 \text{ m} \qquad \text{Eqn. 9c}$$

giving a volume of

$$V_1 = 10.97 \text{ m}^3 \qquad \text{Eqn. 10}$$

For Section 2, we developed an expression for the vertical cross-sectional area, shown in Figure 11, as a function of the location along the width axis. To calculate the volume, we integrated this cross-section to get

$$V_2 = \int A(w)\, dw = 47.50 \text{ m}^3 \qquad \text{Eqn. 11}$$

where the width of Section 2, taken from Figure 9, is

$$W_2 = 8.51 \text{ m} \qquad \text{Eqn. 12}$$

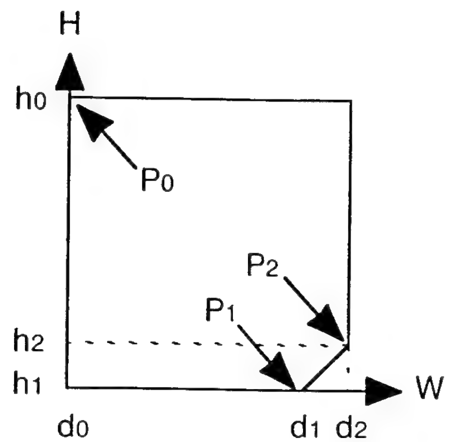

Figure 11. Cross-Section of Laundry Passageway Section 2

The cross sectional area was calculated as a function of the coordinates of the points P_0, P_1 and P_2. The details of this calculation were discussed in reference [7].

4.1.3 Estimation of actual surface areas

As in the case of the Laundry Room, the Laundry Passageway bulkheads were made of several different thicknesses of steel plate. We again created a new material for the thermophysical database that had a thickness equal to the area-weighted mean thickness of the actual materials. In order to calculate this average, we first estimated the areas for each portion of the real bulkheads.

For Section 1, these areas were immediately found from the dimensions

$$A_{deck} = A_{ovhd} = 4.27 \text{ m}^2 \qquad \text{Eqn. 13a}$$

$$A_{fwd} = A_{aft} = 4.50 \text{ m}^2 \qquad \text{Eqn. 13b}$$

$$A_{stbd} = 6.27 \text{ m}^2 \qquad \text{Eqn. 13c}$$

Note that the entire port side of Section 1 is open to Section 2 and, therefore, there is no A_{port}.

In the case of Section 2, the areas of the forward and aft bulkheads were calculated from our cross-section area expression, A(w), using the appropriate values for w. The slanted portion of the port bulkhead area was treated as a trapezoid having two parallel edges the lengths of which were the hypotenuses of the dotted triangles shown in Figure 9. The vertical part of the port bulkhead was also a trapezoid, but had to be split into upper and lower parts because the hull thickness changed at the 1.83 m (6.00 ft) level.

Thus, the surface areas for Section 2 were

$$A_{deck} = 13.66 \text{ m}^2 \qquad \text{Eqn. 14a}$$

$$A_{ovhd} = 19.19 \text{ m}^2 \quad \text{Eqn. 14b}$$

$$A_{fwd} = 5.90 \text{m}^2 \quad \text{Eqn. 14c}$$

$$A_{aft} = 5.26 \text{ m}^2 \quad \text{Eqn. 14d}$$

$$A_{stbd} = 15.60 \text{ m}^2 \quad \text{Eqn. 14e}$$

$$A_{port\ upper} = 6.30 \text{ m}^2 \quad \text{Eqn. 14f}$$

$$A_{port\ lower} = 10.00 \text{ m}^2 \quad \text{Eqn. 14g}$$

$$A_{port\ slant} = 7.84 \text{ m}^2 \quad \text{Eqn. 14h}$$

The deck and overhead were made of the same 0.95 cm (0.375 in.) steel as in the Laundry Room itself (SHIP3/8). The area-weighted mean thickness for the Laundry Passageway bulkhead was calculated to be 1.05 cm (0.414 in.). For reference, Table 4 lists the areas and thicknesses for each part of each surface. The thermal properties database entry for this material was labeled SHIPLRP.

Surface	Section 1		Section 2	
	Area (m2)	Thick (cm)	Area (m2)	Thick (cm)
Adeck	4.27	0.952	13.66	0.952
Aovhd	4.27	0.952	19.19	0.952
Afwd	4.50	0.318	5.90	0.952
Aaft	4.50	0.952	5.26	0.952
Astbd	6.27	1.270	15.60	0.318
Aport,upper	--	--	6.30	1.905
Aport,lower	--	--	10.00	1.588
Aport,slant	--	--	7.84	1.588

Table 4. Laundry Passageway Boundary Areas and Thicknesses

Section 1 has no port bulkhead and the Section 2 port bulkhead is composed of three parts. For the overall compartment, only the total bulkhead area is meaningful.

4.1.4 Approximation of compartment dimensions

We now have estimates for the actual dimensions for Section 1 (Equations 9a - 9e) and for the width of Section 2 (Equation 12); the height and depth of the latter are still to be determined. Since there were no unambiguous values for either of these dimension, we had to use approximate values for both.

Note that most of Section 2 is the same height as Section 1 (2.57 m)[15] and that all of the horizontal vents were in regions with that height. Recalling our discussion of the importance of compartment and soffit heights for horizontal vent flow, we concluded that we could approximate Section 2 as if it all had a height of 2.57 m with minimal error.

Accordingly, we have

$$H_2 = 2.57 \text{ m} \qquad \text{Eqn. 15}$$

and it follows that

$$D_2 = V_2 / (H_2 * W_2) = 2.17 \text{ m} \qquad \text{Eqn. 16}$$

Table 5 summarizes the approximate dimensions that were used for both sections of the Laundry Passageway.

Quantity (units)	Psgwy (Sec 1)	Psgwy (Sec 2)
H (m)	2.57	2.57
W (m)	2.44	8.51
D (m)	1.75	2.17
V (m3)	10.97	47.50

Table 5. Dimensions of Laundry Passageway Section

4.2 Geometrical Simplifications

Based on the approximate compartment dimensions discussed above, two alternative approaches to modeling the Laundry Passageway were developed and tested. One approach was to rearrange the two sections of the compartment to create a single rectangular parallelepiped which could be represented by one set of dimensions. The alternative method involved treating each section of the Laundry Passageway as a separate compartment. We refer to this as the virtual compartment technique because it resulted in the inclusion of an additional compartment in the model – one that does not actually exist.

4.2.1 Rearranging the compartment

Our goal in rearranging the pieces of the Laundry Passageway was to create a set of effective dimensions (H_{eff}, W_{eff} and D_{eff}) which reasonably approximate the compartment.

From Equation 7, the actual Laundry Passageway volume was estimated to be

$$V = 58.47 \text{ m}^3 \qquad \text{Eqn. 17}$$

Since the approximate height of Section 2 was the same as the actual height of Section 1, we chose to use that value as the effective height

$$H_{eff} = 2.57 \text{ m} \qquad \text{Eqn. 18}$$

[15] The exception is the narrow strip, along the port edge of the compartment, where the slanted portion of the hull reduced the effective height.

In order to select values for the effective depth and width, we conceptually reassembled Sections 1 and 2 to create an equivalent geometry. Since CFAST has no knowledge of the actual orientation or position of one compartment relative to another[16], we are free to choose any configuration that is convenient. For our purposes, we chose the arrangement shown in Figure 12. Essentially, we have rotated Section 2 by 90 degrees and attached it to Section 1 so that the width and depth dimensions are swapped. The effective depth of the equivalent compartment is then the actual depth of Section 1 plus the actual width of Section 2. Using values from Table 5, we obtained

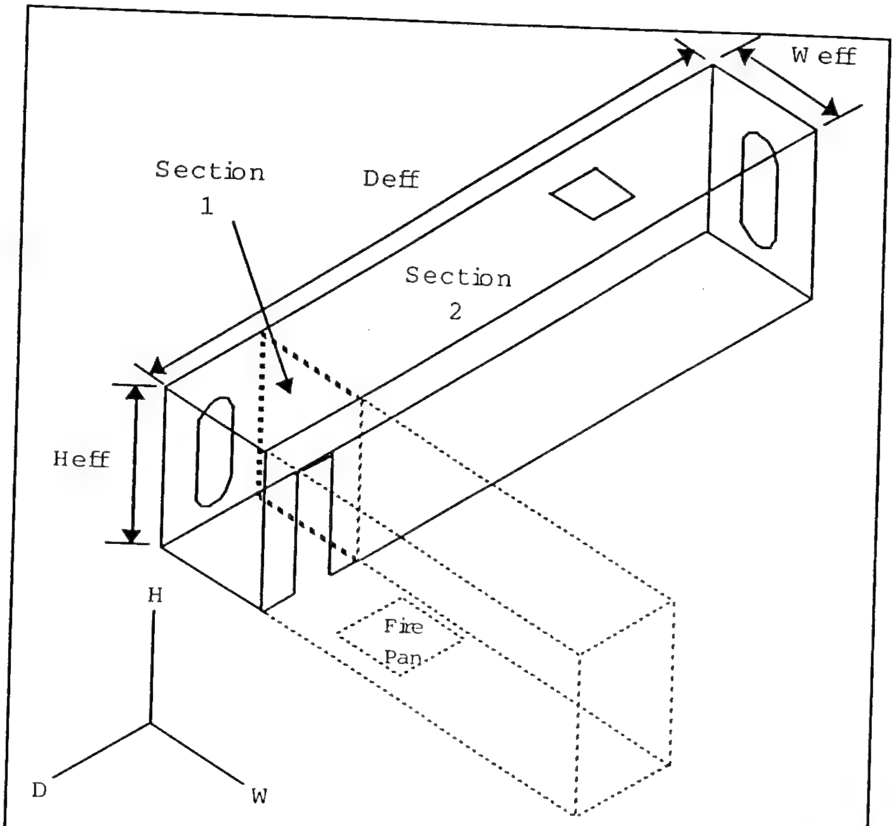

Figure 12. "Rearranged Compartment" Representation of the Laundry Passageway

$$D_{eff} = D_1 + W_2 = 10.26 \text{ m} \qquad \text{Eqn. 19}$$

and the effective width was

$$W_{eff} = V / (H_{eff} * D_{eff}) = 2.22 \text{ m} \qquad \text{Eqn. 20}$$

Combining these dimensions with the information regarding the construction materials and vents from the previous section, we developed the combined Laundry Room/Laundry Passageway geometry given in Listing 6.

[16] The exception to this is that, by using the HI/F and CFCON keywords, it is possible to specify the relative positions of the floors of different compartments.

```
VERSN     3 SHADWELL/688 Laundry Passageway (Rearrangement)
#        Sim.time  Print  Hist.  Disp.  Copies
TIMES      1250      1      3      0      0
#          Temp.     Press.     Elev.
TAMB    285.900   101300.   0.000000
EAMB    286.300   101300.   0.000000
#       Cmpt. 1   Cmpt. 2   Cmpt. 3
#       Laundry    Psgwy    Exterior
#Floor elevation
HI/F    0.00      0.00
#X dimen.
DEPTH   1.75      10.26
#Y dimen.
WIDTH   6.07      2.22
#Z dimen.
HEIGH   2.57      2.57
#Materials
CEILI   SHIP3/8   SHIP3/8
WALLS   SHIPLR    SHIPLRP
FLOOR   SHIP3/8   SHIP3/8
#Laundry-Passageway door
#      Cmpt#    Cmpt#    Vent#    Width     Soffit    Sill    Wind
HVENT  1         2        1        0.66      1.90      0.00    0.00
#      Cmpt#    Cmpt#    Vent#   Width@t0  Width@t1
CVENT  1         2        1       1.00      1.00
#Passageway-AMR door
#      Cmpt#    Cmpt#    Vent#    Width     Soffit    Sill    Wind
HVENT  2         3        1        0.66      2.04      0.23    0.00
#      Cmpt#    Cmpt#    Vent#   Width@t0  Width@t1
CVENT  2         3        1       1.00      1.00
#Passageway-Torpedo Rm door
#      Cmpt#    Cmpt#    Vent#    Width     Soffit    Sill    Wind
HVENT  2         3        2        0.66      2.04      0.23    0.00
#      Cmpt#    Cmpt#    Vent#   Width@t0  Width@t1
CVENT  2         3        2       1.00      1.00
#Passageway-Wardroom hatch
#      Cmpt#    Cmpt#    Area    Type (1 = circular; 2 = square)
VVENT  2         3        0.25      2
#         X       Y      Z
FPOS    0.91   1.83   0.19
#Fire Cmpt
LFBO        1
#Fire Type (1 = unconstrained; 2 = constrained)
LFBT        2
#                  t0        t1
FTIME                      1250.
#Mass pyrolysis rate
FMASS            0.0253    0.0229
#       Mol Wt    Rel Hum    LOL        Hc        Init T    Ign. T    Rad. fract.
CHEMI    184.       100.     10.    4.19E+007    285.9      330.       0.30
#H:C mass ratio (fuel composition)
HCR              0.143      0.143
#O:C mass ratio (fuel composition)
O2               0.0       0.0
```

Listing 6. CFAST Input File for the Laundry Passageway Simulation using the Compartment Rearrangement Method

```
#Soot:CO2 mass ratio (combustion)
OD              0.06     0.06
#CO:CO2 mass ratio (combustion)
CO              0.056    0.056
#HCN:fuel mass ratio (pyrolysis)
HCN             0.0      0.0
#HCl:fuel mass ratio (pyrolysis)
HCL             0.0      0.0
#Toxics:fuel mass ratio (pyrolysis)
CT              0.0      0.0
CJET OFF
DUMPR model.HI
```

Listing 6 (cont'd). CFAST Input File for the Laundry Passageway Simulation using the Compartment Rearrangement Method

4.2.2 Use of virtual compartments

The virtual compartment technique provides more degrees of freedom than does the rearrangement method because each virtual compartment has its own dimensions and vent definitions. This permits the actual relationships among compartments to be more accurately represented. However, it is important to remember that, except for HI/F and CFCON, the current version of CFAST does not include information regarding the actual spatial relationships among compartments. Thus, a carefully crafted representation using virtual compartments may suggest a greater degree of detail than CFAST actually uses.

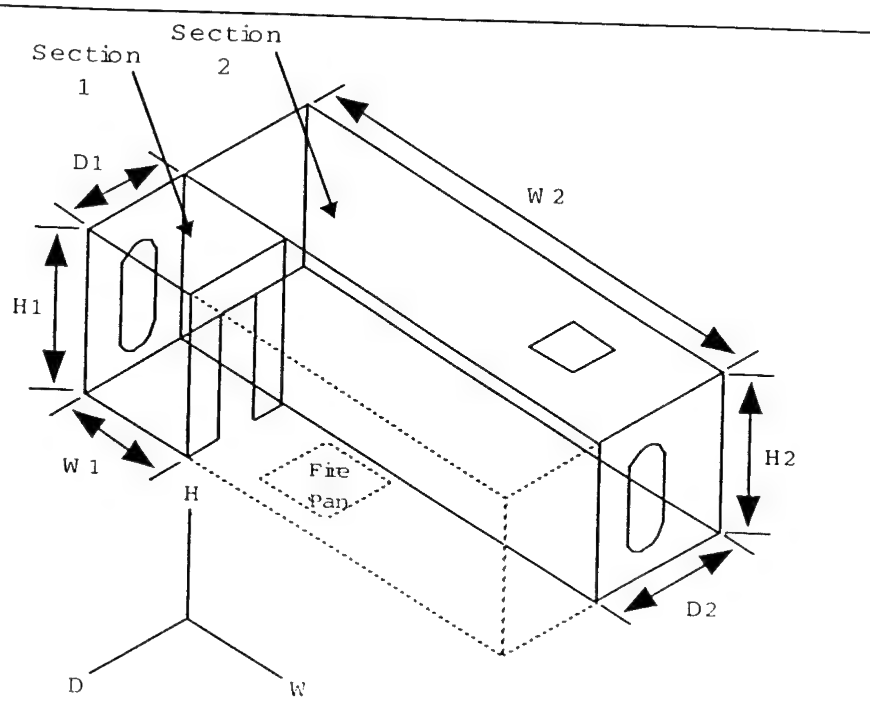

Figure 13. "Virtual Compartment" Representation of the Laundry Passageway

For this approach, we used the dimensions from Table 5 to define two compartments which, taken together, represent the Laundry Passageway. In this model, the fire compartment (Laundry

Room) was compartment one so Sections 1 and 2 of the Laundry Passageway became compartments two and three, respectively.

In this representation, the vertical vent and one of the horizontal vents is located in compartment three and the second horizontal vent is in compartment two. All three connect to the external environment, which is now compartment four. Finally, a new horizontal vent was defined to represent the entire 2.44 m (8.01 ft) x 2.57 m (8.43 ft) bulkhead between the two sections. The equivalent geometry of this layout is shown in Figure 13.

The area-weighted bulkhead thicknesses were recalculated, using the values from Table 4, to be 0.0090 cm (0.353 in.) and 0.0110 cm (0.433 in.) for compartments two and three, respectively. Two new entries, SHIPLRP1 and SHIPLRP2, were defined in the Thermal.df file to represent these materials. The resulting model geometry is shown in Listing 7.

```
VERSN     3 SHADWELL/688 Laundry Passageway (Virtual)
#         Sim.time  Print   Hist.   Disp.   Copies
TIMES       1250      1       3       0       0
#           Temp.      Press.      Elev.
TAMB     285.900    101300.    0.000000
EAMB     286.300    101300.    0.000000
#        Cmpt. 1    Cmpt. 2    Cmpt. 3
#        Laundry    Psgwy 1    Psgwy 2    Exterior
#Floor elevation
HI/F     0.00       0.00       0.00
#X dimen.
DEPTH    1.75       1.75       2.17
#Y dimen.
WIDTH    6.07       2.44       8.51
#Z dimen.
HEIGH    2.57       2.57       2.57
#Materials
CEILI    SHIP3/8    SHIP3/8    SHIP3/8
WALLS    SHIPLR     SHIPLRP1   SHIPLRP2
FLOOR    SHIP3/8    SHIP3/8    SHIP3/8
#Laundry-Psgwy 1 door
#       Cmpt#    Cmpt#    Vent#    Width      Soffit    Sill    Wind
HVENT   1        2        1        0.66       1.90      0.00    0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT   1        2        1        1.00       1.00
#Psgwy 1-AMR door
#       Cmpt#    Cmpt#    Vent#    Width      Soffit    Sill    Wind
HVENT   2        4        1        0.66       2.04      0.23    0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT   2        4        1        1.00       1.00
#Psgwy 1-Psgwy 2 door
#       Cmpt#    Cmpt#    Vent#    Width      Soffit    Sill    Wind
HVENT   2        3        1        2.44       2.57      0.00    0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT   2        3        1        1.00       1.00
#Psgwy 2-Torpedo Rm door
#       Cmpt#    Cmpt#    Vent#    Width      Soffit    Sill    Wind
HVENT   3        4        1        0.66       2.04      0.23    0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT   3        4        1        1.00       1.00
```

Listing 7. CFAST Input File for the Laundry Passageway Simulation using the Virtual Compartment Method

```
#Passageway-Wardroom hatch
#       Cmpt#    Cmpt#    Area    Type (1 = circular; 2 = square)
VVENT   3        4        0.78      2
#         X        Y        Z
FPOS    0.91    1.83    0.19
#Fire Cmpt
LFBO        1
#Fire Type (1 = unconstrained; 2 = constrained)
LFBT        2
#                    t0          t1
FTIME                            1250.
#Mass pyrolysis rate
FMASS               0.0253      0.0229
#        Mol Wt    Rel Hum     LOL          Hc         Init T     Ign. T    Rad. fract.
CHEMI     184.        100.      10.    4.19E+007     285.9       330.        0.30
#H:C mass ratio (fuel composition)
HCR                 0.143        0.143
#O:C mass ratio (fuel composition)
O2                  0.0          0.0
#Soot:CO2 mass ratio (combustion)
OD                  0.06         0.06
#CO:CO2 mass ratio (combustion)
CO                  0.056        0.056
#HCN:fuel mass ratio (pyrolysis)
HCN                 0.0          0.0
#HCl:fuel mass ratio (pyrolysis)
HCL                 0.0          0.0
#Toxics:fuel mass ratio (pyrolysis)
CT                  0.0          0.0
CJET OFF
DUMPR model.HI
```

Listing 7 (cont'd). CFAST Input File for the Laundry Passageway Simulation using the Virtual Compartment Method

4.3 Problems of Vertical Transport

CFAST incorporates vertical transport in two different ways: 1) mass transport through vertical vents and 2) upward conduction between two vertically adjacent compartments. The former aspect was first encountered when the vertical vent in the Laundry Passageway was included in the model.

By default, CFAST assumes that the "back" side of any boundary is exposed to the external environment. This means that the ambient temperature, rather than the temperature of another compartment, is used for conduction calculations. It also means that energy is transferred to the external environment instead of into the second compartment. For the Laundry Passageway model this behavior was correct — the far side of the overhead was the exterior. However, when the Wardroom was added, compartment-to-compartment vertical conduction became a factor and the default behavior was no longer appropriate.

In the follow two sections, we discuss the problems observed with both of these vertical transport mechanisms and present possible solutions.

4.3.1 Vertical mass transport

The Laundry Passageway vertical vent was rectangular, with dimensions of 0.96 m (3.15 ft) by 0.81 m (2.66 ft). Because CFAST limits VVENTs to circles or squares, we had to approximate this as a square, which was reasonably close to the actual shape. The vent area was defined to be equal to that of the actual hatch, 0.78 m^2 (8.40 ft^2).

The hatch described above was included in both the "rearranged geometry" and the "virtual compartment" versions of the Laundry Passageway model. In both cases, we found that the model failed to run to the end of the 1250 second simulation. When the "rearranged geometry" approach was used, the model ran at normal speeds for the first 148 seconds of the simulation (at a rate of about four simulated seconds per second of computer time[17]) but then the execution speed dropped four orders of magnitude (to approximately 3 simulated milliseconds per second). With the virtual compartment model, CFAST stalled after only 78 seconds of simulation. At those rates, the model is effectively unusable because, on typical desktop computers, it would take days to complete each simulation.

The stalling problem is a consequence of the way in which CFAST calculates the size of the time step to be used by the numerical solver. The step size is adjusted, upward or downward, based on the results of previous steps. The step size is increased when convergence is reached very quickly and decreased if convergence fails. Typically, the step size is on the order of milliseconds (it can be as much as several seconds when conditions are especially favorable) but, after repeated convergence failures, the step size can be reduced to a fraction of a microsecond. Under normal circumstances, simulating one second requires only hundreds or thousands of iterations but this can grow to tens of millions of iterations under adverse conditions.

When faced with stalling problems, the first step is to determine which keywords are involved[18]. The easiest way to accomplish this is to "comment out" the suspect lines, one at a time, by inserting a pound sign (#) as the first character in the line. If the model no longer stalls, then some parameter associated with that keyword was a contributing factor.

Assuming that VVENT has been so identified, there are several possible methods for resolving the problem. The first is to try different vent areas or shapes until a combination is found which permits the model to run to completion. It is then the responsibility of the user to determine whether the resulting parameters adequately represent the actual situation. If they do not, then the only recourse is to identify additional interacting keywords or parameters and make adjustments to them.

Using the compartment rearrangement method, we found that the Laundry Passageway model ran for the full simulation period if the area of the VVENT was less than about 0.25 m^2 (2.69 ft^2) or greater than approximately 7.5 m^2 (66.2 ft^2). With the virtual compartment technique, serious stalling problems were noted for all non-zero vent areas. These results are illustrated in Figures 14 and 15, which show the completion fraction, as a function of vent area, for the two different

[17] Typical execution rates on current microcomputers are on the order of 10 simulated seconds per second. However, the solver is slower at the beginning of the simulation because it is making essentially random guesses. Once it has acquired a history of prior solutions, the solver predictions get better and it speeds up. Transient inputs (a step function change in burning rate, for example) normally cause a temporary slowdown until a new history can be developed. Also, CFAST requires several minutes to load and initialize. Since this disproportionately affects short simulations, we did not begin timing until after the startup delay.

[18] Runtime problems with CFAST are usually due to interactions among parameters associated with multiple keywords. Therefore, it is not generally correct to say that a specific parameter or keyword is the cause of the difficulties.

approaches. Completion fraction is defined as the number of simulated seconds prior to stalling divided by the total planned simulation time (1250 seconds).

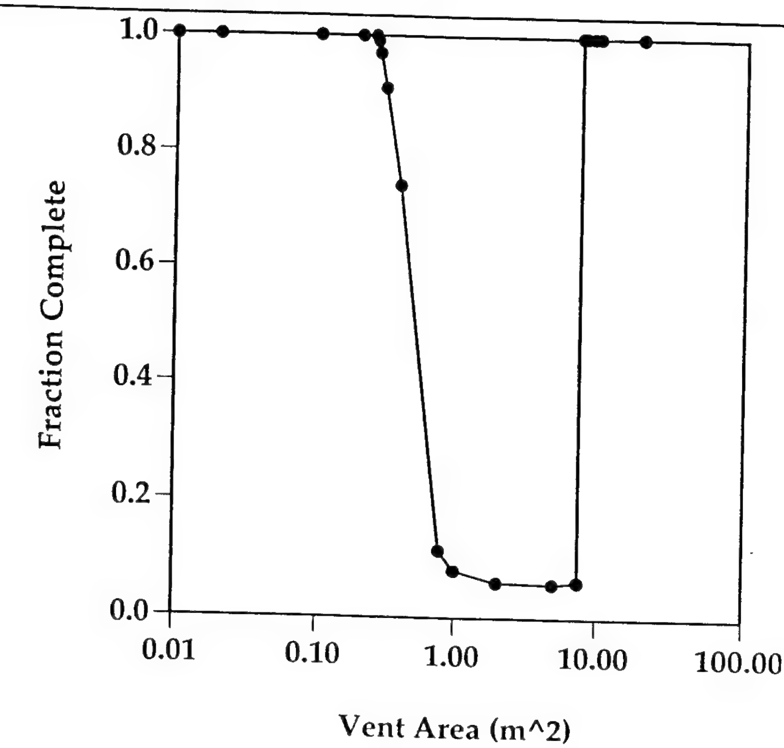

Figure 14. Completion Fraction for Compartment Rearrangement Model

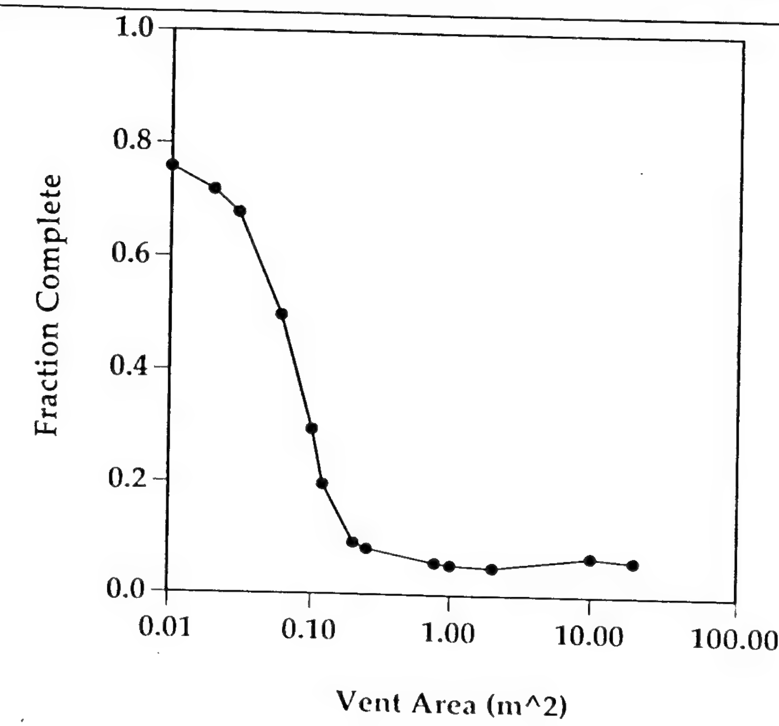

Figure 15. Completion Fraction for Virtual Compartment Model

It became apparent that, if we used the virtual compartment method, we would have to eliminate the Laundry Passageway-Wardroom hatch from the model. Since it was obvious that the model predictions for the Wardroom would be grossly incorrect without that hatch, we chose not to pursue the virtual compartment approach any further for this work. We must note, however, that the fact that virtual compartments were inappropriate in this specific case does not indicate that they could not be useful in other cases.

We have found that stalling problems sometimes vanish if the dimensions of one of the connected compartments is changed. For example, our difficulties with the Laundry Passageway VVENT were eliminated when the Wardroom was added. The effect of this addition was to change the destination compartment from the essentially infinite volume of the exterior to a finite volume.

Adding the Wardroom might also have made it possible to use virtual compartments. Unfortunately, there are so many possible approximations for complex models that combinatorial explosion becomes a problem — it is impossible to exhaustively investigate all combinations and the user must prune entire branches from the possibility tree. In our case, we elected not to pursue the virtual compartment approach and, instead, used compartment rearrangement. The vent area was set to 0.25 m^2 (2.69 ft^2) because that was the closest we could get to the actual hatch area.

4.3.2 Vertical heat conduction

By default, CFAST does not know that the overhead of one compartment is the deck of another. Therefore, heat conduction between two vertically adjacent compartments is normally not calculated. However, the CFCON keyword can be used to inform CFAST that a particular pair of compartments is vertically adjacent. When used, this keyword enables vertical heat transfer from the lower compartment to the upper[19]. Modeling of the Wardroom provided an example of the application of vertical heat conduction.

Since the Wardroom overlies both the Laundry Room and the Laundry Passageway, the obvious approach was to connect both lower-deck compartments to the Wardroom. Unfortunately, this did not work — if two CFCON inputs to the same compartment are specified, the numerical solver fails to initialize properly and causes CFAST to immediately quit[20]. Consequently, in cases like this, the user must determine which one of the possible connections is the most important and which can safely be neglected.

We investigated both possibilities: conduction between Laundry and Wardroom and between Laundry Passageway and Wardroom. There was an interaction between the Wardroom-exterior vent (VVENT) and the Laundry-Wardroom or Laundry Passageway-Wardroom conduction (CFCON). In either case, when the correct area [0.78 m^2 (8.40 ft^2)] of the exterior vertical vent was specified, there were stalling problems similar to those previously discussed. Without vertical conduction, the model ran correctly with the actual vent area. By trial and error, it was discovered that the model would run for either conduction configuration if the exterior vent size was reduced to 0.26 m^2 (2.80 ft^2) or below.

We chose to use conduction between the Laundry Room and the Wardroom for two reasons: 1) conduction from the Laundry was greater than conduction from the Laundry Passageway

[19] CFCON changes the behavior of vertical conduction (through overheads/decks) to permit energy to be added to the upper compartment. It does not affect horizontal heat conduction (through bulkheads).
[20] It is acceptable for one compartment to have both a conductive input (through the deck) and an output (through the overhead).

because the former was much hotter; and 2) the vertical vent already provided a transport path from the Laundry Passageway. Listing 8 shows the final version of the Wardroom input file.

```
VERSN     3 SHADWELL/688 Laundry - Wardroom
#         Sim.time  Print  Hist.  Disp.  Copies
TIMES       1250      1      3      0      0
#          Temp.     Press.     Elev.
TAMB     285.900   101300.   0.000000
EAMB     286.300   101300.   0.000000
#        Cmpt. 1   Cmpt. 2   Cmpt. 3    Cmpt. 4
#        Laundry   Psgwy     Wardroom   Exterior
#Floor elevation
HI/F     0.00      0.00      2.57
#X dimen.
DEPTH    1.75      10.26     4.00
#Y dimen.
WIDTH    6.07      2.22      8.51
#Z dimen.
HEIGH    2.57      2.57      2.59
#Materials
CEILI    SHIP3/8   SHIP3/8   SHIP7/8
WALLS    SHIPLR    SHIPLRP   SHIPWR
FLOOR    SHIP3/8   SHIP3/8   SHIP3/8
#Laundry-Passageway door
#      Cmpt#    Cmpt#    Vent#    Width      Soffit     Sill    Wind
HVENT  1        2        1        0.66       1.90       0.00    0.00
#      Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT  1        2        1        1.00       1.00
#Passageway-AMR door
#      Cmpt#    Cmpt#    Vent#    Width      Soffit     Sill    Wind
HVENT  2        4        1        0.66       2.04       0.23    0.00
#      Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT  2        4        1        1.00       1.00
#Passageway-Torpedo Rm door
#      Cmpt#    Cmpt#    Vent#    Width      Soffit     Sill    Wind
HVENT  2        4        2        0.66       2.04       0.23    0.00
#      Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT  2        4        2        1.00       1.00
#Passageway-Wardroom hatch
#      Cmpt#    Cmpt#    Area     Type (1 = circular; 2 = square)
VVENT  2        3        0.78       2
#Wardroom-Crew Mess door
#      Cmpt#    Cmpt#    Vent#    Width      Soffit     Sill    Wind
HVENT  3        4        1        0.66       2.04       0.23    0.00
#      Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT  3        4        1        1.00       1.00
#Wardroom-Crew Living door
#      Cmpt#    Cmpt#    Vent#    Width      Soffit     Sill    Wind
HVENT  3        4        2        0.66       2.04       0.23    0.00
#      Cmpt#    Cmpt#    Vent#    Width@t0   Width@t1
CVENT  3        4        2        1.00       1.00
#Wardroom-Nav. Equip. Room hatch
#      Cmpt#    Cmpt#    Area     Type (1 = circular; 2 = square)
VVENT  3        4        0.26       2
#      Cmpt#    Cmpt#
```

Listing 8. CFAST Input File for the Wardroom Simulation

```
CFCON    1        3
#           X      Y      Z
FPOS    0.91  1.83  0.19
#Fire Cmpt
LFBO      1
#Fire Type (1 = unconstrained; 2 = constrained)
LFBT      2
#                t0       t1
FTIME                    1250.
#Mass pyrolysis rate
FMASS           0.0253   0.0229
#      Mol Wt   Rel Hum   LOL        Hc       Init T   Ign. T  Rad. fract.
CHEMI    184.      100.   10.   4.19E+007   285.9     330.     0.30
#H:C mass ratio (fuel composition)
HCR             0.143     0.143
#O:C mass ratio (fuel composition)
O2              0.0      0.0
#Soot:CO2 mass ratio (combustion)
OD              0.06     0.06
#CO:CO2 mass ratio (combustion)
CO              0.056     0.056
#HCN:fuel mass ratio (pyrolysis)
HCN             0.0      0.0
#HCl:fuel mass ratio (pyrolysis)
HCL             0.0      0.0
#Toxics:fuel mass ratio (pyrolysis)
CT              0.0      0.0
CJET OFF
DUMPR model.HI
```

Listing 8 (cont'd). CFAST Input File for the Wardroom Simulation

4.4 Problems of Ambiguous Thermophysical Properties

We have seen, in both the Laundry Room and the Laundry Passageway, that it is necessary to create fictitious materials in cases where the actual bulkheads are composed of patches of different materials[21]. In the previous cases, this problem was relatively simple because the patches had the same composition and differed only in thickness. The Navigation Equipment Room (Figure 16) was much more complex because the bulkheads differed in composition as well as in thickness.

All of the original bulkheads in the Navigation Equipment Room were composed of various thicknesses of steel. However, the forward bulkhead (on the right in Figure 16) was a temporary partition made of plywood. The thermal conductivities, heat capacities and densities of steel and plywood are vastly different and it was not immediately obvious what weighting factors should be used to calculate meaningful average values.

For consistency with our prior work, we used area-weighting to calculate the mean thickness and this thickness was used for all subsequent calculations. For the conductivity, we required that the effective heat flux, Q, be equal to the sum of the actual heat fluxes, Q_i, through the various pieces of the bulkhead

$$Q = \sum Q_i \qquad \text{Eqn. 21}$$

[21] This rule also applies to deck and overhead boundaries, although there were no such examples in this case study.

or, in terms of the material properties,

$$\kappa A \Delta T / t = \sum \kappa_i A_i \, \Delta T_i / t_i \qquad \text{Eqn. 22}$$

where κ, A and t are conductivity, area and thickness and ΔT is the temperature difference across the thickness. The subscripts refer to the sections of the bulkhead; unsubscripted values refer to the effective values for our approximated compartment.

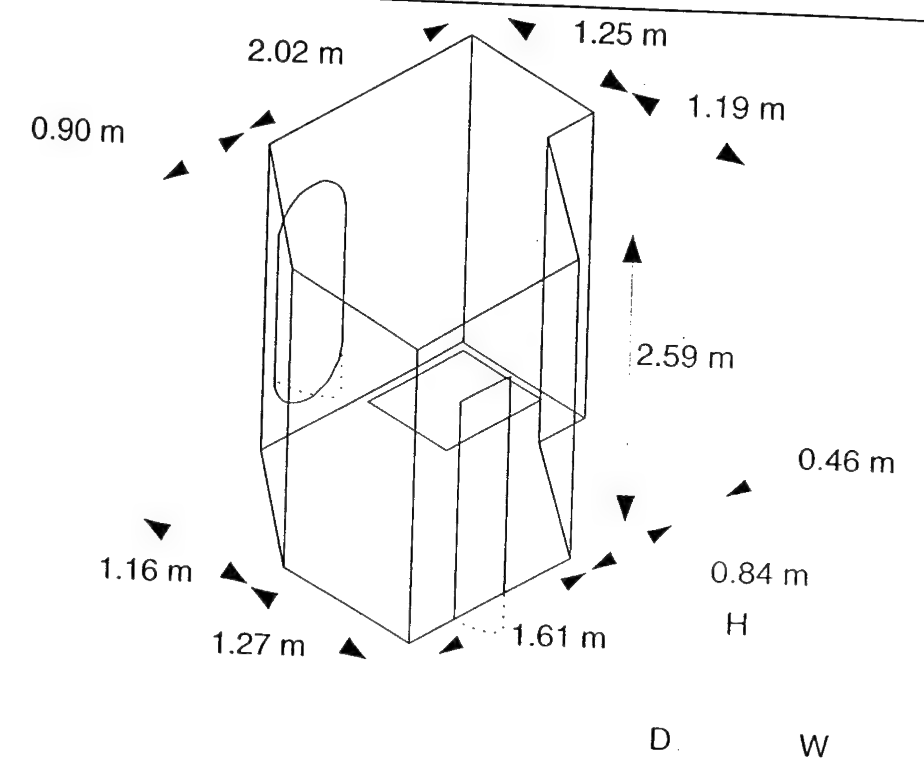

Figure 16. Navigation Equipment Room Dimensions

In general, each part of the real bulkhead may have a different ΔT_i and, since those values are time dependent, we cannot calculate a constant value for the effective conductivity. Recall, however, that the current version of CFAST treats walls as if they were a single entity that wraps around the compartment. Due to this limitation, CFAST acts as though all of the ΔT_i values were the same. Consequently, we introduce no additional error if we also treat ΔT_is as if they were the same for all parts of the bulkhead. Using this approximation, we can cancel the temperature terms on both sides of Equation 22 and, solving for κ, we get

$$\kappa = \sum \kappa_i (A_i / A)(t / t_i) \qquad \text{Eqn. 23}$$

The derivation of the weighting factors for thickness assumed that the total mass of the approximated bulkheads was equal to the total mass of the real bulkheads. Applying this assumption to the density, and using the approach illustrated above, gives us

$$\rho = \sum \rho_i (A_i / A)(t_i / t) \qquad \text{Eqn. 24}$$

Similarly, the requirement for equal heat content of the bulkheads leads to

$$C = \sum C_i (\rho_i / \rho)(A_i / A)(t_i / t) \qquad \text{Eqn. 25}$$

In order to apply these equations, we first calculated the areas of the seven parts of the Navigation Equipment Room bulkhead (indicated by the circled numbers in Figure 17) using the compartment dimensions from Figure 16. The area-weighted thickness was then calculated and, with this information, we were able to determine all of the weighting factors for Equations 23 - 25. Standard values for the thermophysical properties of steel and plywood were taken from the default Thermal.df file (the relevant portion of which is shown in Table 6). The calculated mean property values for the fictitious material (SHIPNER) are given in Table 7.

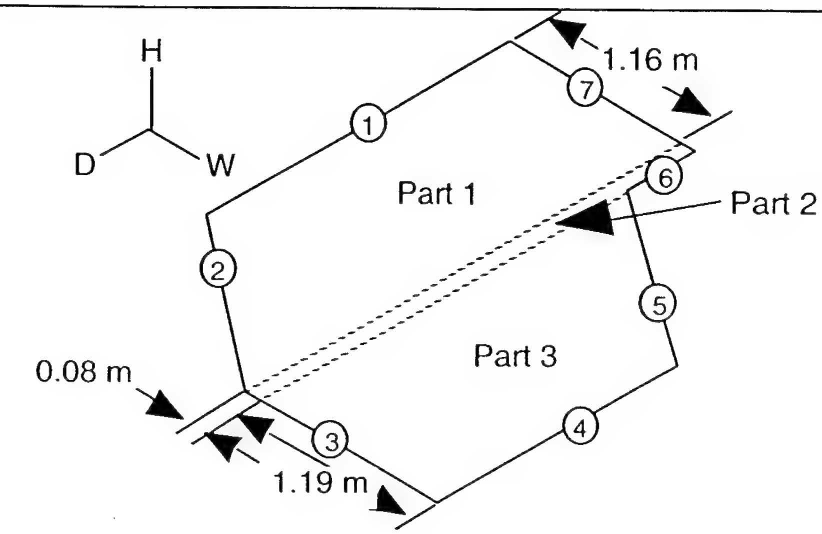

Figure 17. Division of the Navigation Equipment Room Deck into Parts

The deck area was calculated as the sum of the areas of the three parts illustrated. In order to estimate mean values for the thermophysical properties, the bulkhead was divided into seven segments, as indicated by the circled numbers. The area of each segment was the length of the line segment multiplied by the compartment height.

Material	Conductivity (W/m K)	Heat Capacity (J/kg K)	Density (kg/m3)
Steel	48	559	7854
Plywood	0.12	1215	545

Table 6. Standard Thermal.df Entries for Steel and Plywood

Part	Area (m2)	Thick (m)	(A_i / A)	$(A_i / A) t_i$
1	5.23	0.0095	0.2117	0.0020
2	3.81	0.0095	0.1542	0.0015
3	3.29	0.0095	0.1331	0.0013
4*	4.17	0.0127	0.1688	0.0021
5*	3.78	0.0127	0.1530	0.0019
6*	1.19	0.0127	0.0482	0.0006
7	3.24	0.0095	0.1311	0.0012
Totals	24.71			0.0106

Table 7. Calculation of Thermal Properties for SHIPNER

Parts were numbered counterclockwise, starting from the far left of Figure 17. Parts marked with * are plywood; the others are steel.

Part	(t_i / t)	$(A_i t / A t_i) \kappa_i$	$(A_i t_i / At) \rho_i$	$(A_i t_i \rho_i / A t \rho) C_i$
1*	0.8962	11.34	1490	178
2*	0.8962	8.26	1085	130
3*	0.8962	7.13	937	112
4	1.1981	0.0169	110	29
5	1.1981	0.0153	100	26
6	1.1981	0.0048	31	8
7*	0.8962	7.02	923	110
Totals		33.79	4676	593

Table 7 (Cont'd). Calculation of Thermal Properties for SHIPNER

4.5 Results of the Geometry Specification Development

We previously compared Laundry Room temperature predictions, based on our fire specification, to data from the SHADWELL/688 test [6]. In that case, it was relatively easy to separate the portion of the model that was directly affected by the fire specification (the Laundry Room) from the portions that were not (everything else). However, for the geometry specification, the interactions among the various parts of the model make such a simple separation impossible[22].

For example, conditions in the Laundry Passageway clearly depend, in part, on vertical transport (both vent flow and conduction) but that cannot be properly simulated until the Wardroom has been added to the model. Thus, although we have discussed issues such as non-rectangular

[22] Of course, even for the fire specification, this was only an approximation — as will be shown, the addition of the Laundry Passageway changed the predictions for the Laundry Room.

geometry, vertical transport and thermophysical properties as if they were independent, in fact, they are not independent. Accordingly, in this section, we compare the results of modeling the entire domain (Listing 9), rather than subsections of the domain, with the test data. Even then, the predictions can only be considered to be estimates because our model domain did not include the entire SHADWELL/688 test area. As is likely to be true for most real world applications, the model domain was chosen to include the factors of primary interest (in this case, the effects of Laundry Room fires on Control Room habitability) while neglecting other factors (such as the effects on the AMR, Torpedo Room and other compartments).

```
VERSN     3 SHADWELL/688 Laundry - Sail.
#        Sim.time  Print  Hist.  Disp.  Copies
TIMES      1250      1      3      0      0
#          Temp.     Press.     Elev.
TAMB    285.900   101300.   0.000000
EAMB    286.300   101300.   0.000000

#      Cmpt. 1  Cmpt. 2  Cmpt. 3  Cmpt. 4  Cmpt. 5  Cmpt. 6  Cmpt. 7
#      Laundry  Psgwy    Wardrm   NER      CR       Sail_1   Sail_2
#Floor elevation
HI/F    0.00     0.00     2.57     5.16     5.16     7.75     10.18
#X dimen.
DEPTH   1.75     10.26    4.00     2.92     2.90     1.21     0.91
#Y dimen.
WIDTH   6.07     2.22     8.51     1.90     6.30     1.42     0.91
#Z dimen.
HEIGH   2.57     2.57     2.59     2.59     2.59     2.43     1.02

#Materials
CEILI   SHIP3/8  SHIP3/8 SHIP7/8  SHIP3/8  SHIP3/8  SHIP3/8  SHIP3/8
WALLS   SHIPLR   SHIPLRP SHIPWR   SHIPNER  SHIPCR   SHIP3/8  SHIP3/8
FLOOR   SHIP3/8  SHIP3/8 SHIP3/8  SHIP7/8  SHIP7/8  SHIP3/8  SHIP3/8

#Laundry-Passageway door
#       Cmpt#    Cmpt#    Vent#    Width     Soffit    Sill    Wind
HVENT   1        2        1        0.66      1.90      0.00    0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0  Width@t1
CVENT   1        2        1        1.00      1.00

#Passageway-AMR door
#       Cmpt#    Cmpt#    Vent#    Width     Soffit    Sill    Wind
HVENT   2        8        1        0.66      2.04      0.23    0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0  Width@t1
CVENT   2        8        1        1.00      1.00
#Passageway-Torpedo Rm door
#       Cmpt#    Cmpt#    Vent#    Width     Soffit    Sill    Wind
HVENT   2        8        2        0.66      2.04      0.23    0.00
#       Cmpt#    Cmpt#    Vent#    Width@t0  Width@t1
CVENT   2        8        2        1.00      1.00
#Passageway-Wardroom hatch
#       Cmpt#    Cmpt#    Area     Type (1 = circular; 2 = square)
VVENT   2        3        0.78     2
#Wardroom-Crew Mess door
#       Cmpt#    Cmpt#    Vent#    Width     Soffit    Sill    Wind
HVENT   3        8        1        0.66      2.04      0.23    0.00
```

Listing 9. File for the Final SHADWELL/688 Simulation

```
#       Cmpt#    Cmpt#    Vent#   Width@t0   Width@t1
CVENT   3        8        1       1.00       1.00
#Wardroom-Crew Living door
#       Cmpt#    Cmpt#    Vent#   Width      Soffit     Sill     Wind
HVENT   3        8        2       0.66       2.04       0.23     0.00
#       Cmpt#    Cmpt#    Vent#   Width@t0   Width@t1
CVENT   3        8        2       1.00       1.00
#Wardroom-Nav. Equip. Rm. hatch
#       Cmpt#    Cmpt#    Area    Type (1 = circular; 2 = square)
VVENT   3        4        0.78     2
#Laundry-Wardroom heat conduction
#       Cmpt#    Cmpt#
CFCON   1        3

#Nav. Equip. Rm-Fan Rm. door
#       Cmpt#    Cmpt#    Vent#   Width      Soffit     Sill     Wind
HVENT   4        8        1       0.66       2.04       0.23     0.00
#       Cmpt#    Cmpt#    Vent#   Width@t0   Width@t1
CVENT   4        8        1       1.00       1.00
#Nav. Equip. Rm.-Control Rm. door
#       Cmpt#    Cmpt#    Vent#   Width      Soffit     Sill     Wind
HVENT   4        5        1       0.50       1.92       0.00     0.00
#       Cmpt#    Cmpt#    Vent#   Width@t0   Width@t1
CVENT   4        5        1       1.00       1.00

#Control Rm.-Combat Systems door
#       Cmpt#    Cmpt#    Vent#   Width      Soffit     Sill     Wind
HVENT   5        8        1       0.66       2.04       0.23     0.00
#       Cmpt#    Cmpt#    Vent#   Width@t0   Width@t1
CVENT   5        8        1       1.00       1.00
#Control Rm.-Sail_1 hatch
#       Cmpt#    Cmpt#    Area    Type (1 = circular; 2 = square)
VVENT   5        6        0.33     1
#Wardroom-Control Rm. heat conduction
#       Cmpt#    Cmpt#
CFCON   3        5

#Sail_1-Sail_2 opening
#       Cmpt#    Cmpt#    Area    Type (1 = circular; 2 = square)
VVENT   6        7        0.82     1
#Control Rm.-Sail_1 heat conduction
#       Cmpt#    Cmpt#
CFCON   5        6

#Sail_2-Exterior opening
#       Cmpt#    Cmpt#    Area    Type (1 = circular; 2 = square)
VVENT   7        8        0.82     1
#Sail_1-Sail_2 heat conduction
#       Cmpt#    Cmpt#
CFCON   6        7
FPOS    0.91  1.83  0.19
#Fire Cmpt
LFBO         1
#Fire Type (1 = unconstrained; 2 = constrained)
LFBT         2
```

Listing 9 (cont'd). File for the Final SHADWELL/688 Simulation

```
#                  t0       t1
FTIME                       1250.
#Mass pyrolysis rate
FMASS            0.0253   0.0229
#        Mol Wt    Rel Hum    LOL        Hc        Init T    Ign. T   Rad. fract.
CHEMI    184.       100.      10.    4.19E+007     285.9     330.       0.30
#H:C mass ratio (fuel composition)
HCR              0.143     0.143
#O:C mass ratio (fuel composition)
O2               0.0       0.0
#Soot:CO2 mass ratio (combustion)
OD               0.06      0.06
#CO:CO2 mass ratio (combustion)
CO               0.056     0.056
#HCN:fuel mass ratio (pyrolysis)
HCN              0.0       0.0
#HCl:fuel mass ratio (pyrolysis)
HCL              0.0       0.0
#Toxics:fuel mass ratio (pyrolysis)
CT               0.0       0.0
CJET OFF
DUMPR model.HI
```

Listing 9 (cont'd). File for the Final SHADWELL/688 Simulation

The primary purpose of this section is to provide some insights regarding the accuracy of CFAST predictions. It is important to note that good agreement (or lack thereof) in our test case does not guarantee that all simulations will be equally accurate (or inaccurate). Data from the various compartments were processed as previously described and the layer assignments for the thermocouples were again based on the interface heights predicted by CFAST. Since it was not practical to apportion sensors on a second-by-second basis, we used the mean of the interface heights at 60 and 1250 seconds. These times were arbitrary, but approximately represented the period over which the interface height was nearly constant. Table 8 shows the number of thermocouples for both layers of each compartment and the interface heights for all compartments[23] are shown in Figure 18.

Cmpt.	Interface Ht (m)	Upper TCs	Lower TCs
Laundry	0.56	4	2
Passageway	1.54	2	4
Wardroom	1.64	9	20
Nav. Equip.	0.86	4	2
Control Rm.	1.33	6	7

Table 8. Interface Heights and Apportionment of Thermocouples

The number of thermocouples in each layer of each compartment was determined based on the interface heights predicted by CFAST.

[23] The Sail was not included because there was only a single thermocouple in the entire access trunk.

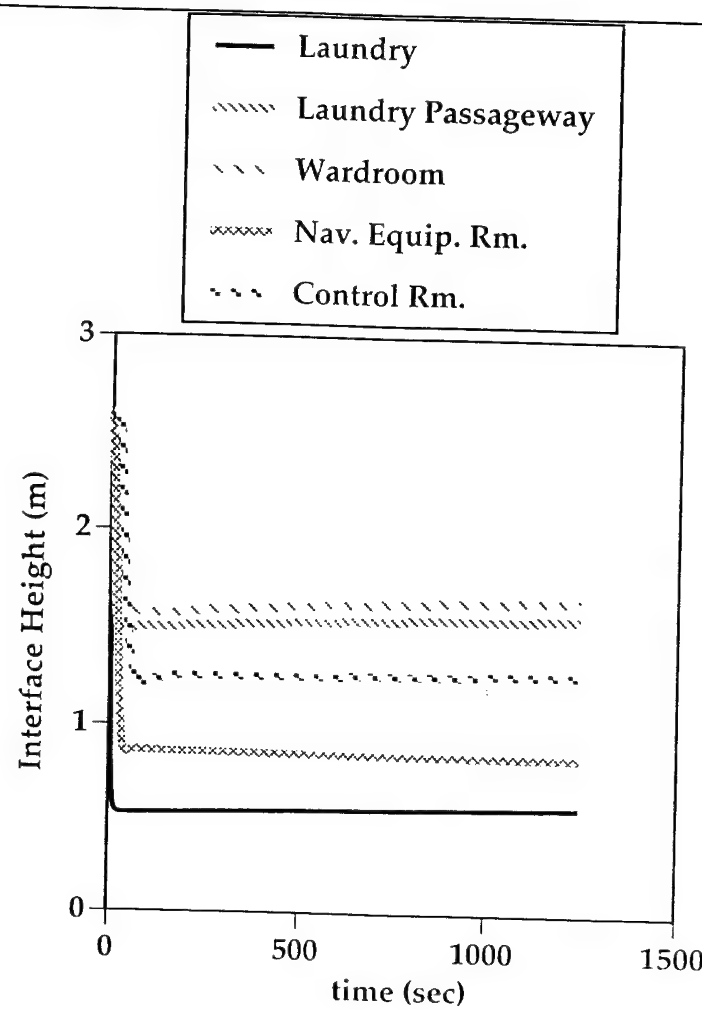

Figure 18. Compartment Interface Heights

These CFAST-predicted interface heights were used to determine which thermocouples were in the upper or lower layers.

Figures 19 - 23 compare the predicted upper and lower layer temperatures with the experimental values for the Laundry Room, Laundry Passageway, Wardroom, Navigation Equipment Room and Control Room. There was excellent agreement between the predicted and actual air temperatures for the Laundry Room itself. The effects of adding additional compartments to the model may be seen by comparing these Laundry Room results with those previously reported (Figure 8).

In the case of the Laundry Passageway, temperatures in both layers were underestimated. For the upper layer, the discrepancy was very large — on the order of five standard deviations. This may be attributed, in part, to measurement errors. The two upper layer thermocouples probably were not a good sample of the temperatures throughout the layer because both were exposed to the gas jet from the Laundry Room and both were located far from the overhead vent leading to the Wardroom. As a result, it is likely that the measured upper layer temperatures were higher that the mean layer temperature.

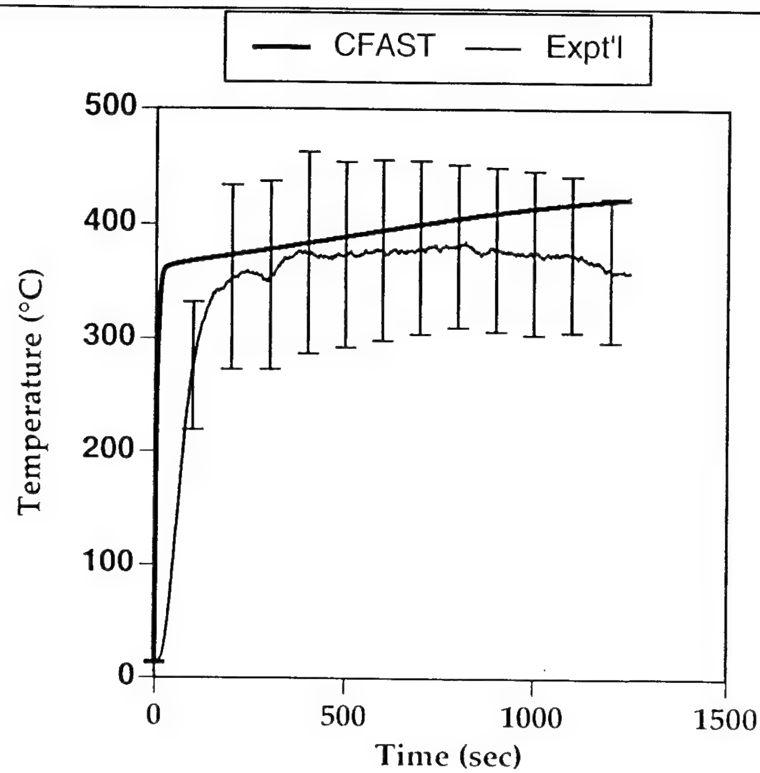

Figure 19A. Predicted versus Measured Laundry Room Upper Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

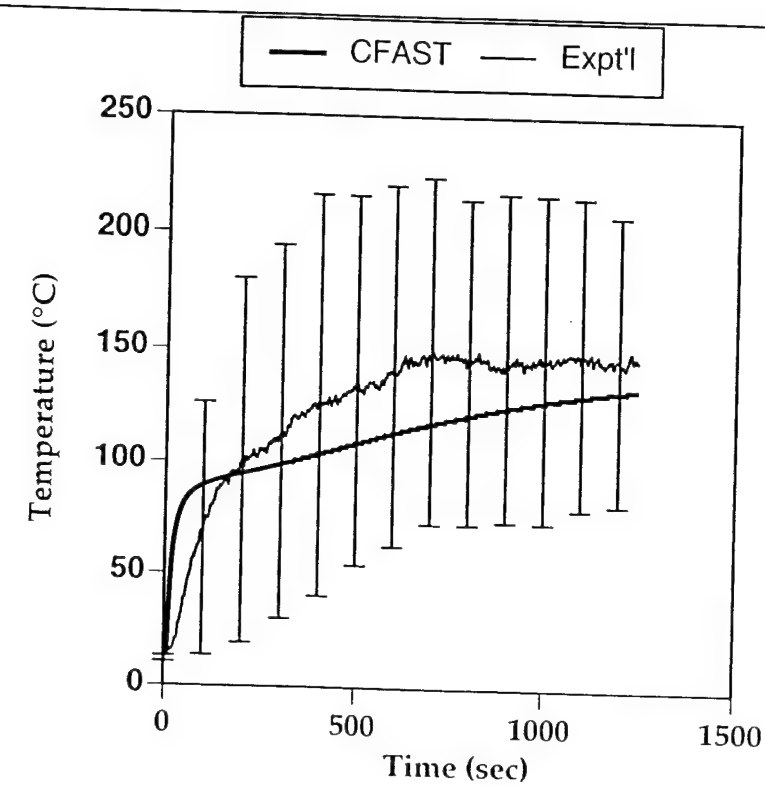

Figure 19B. Predicted versus Measured Laundry Room Lower Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

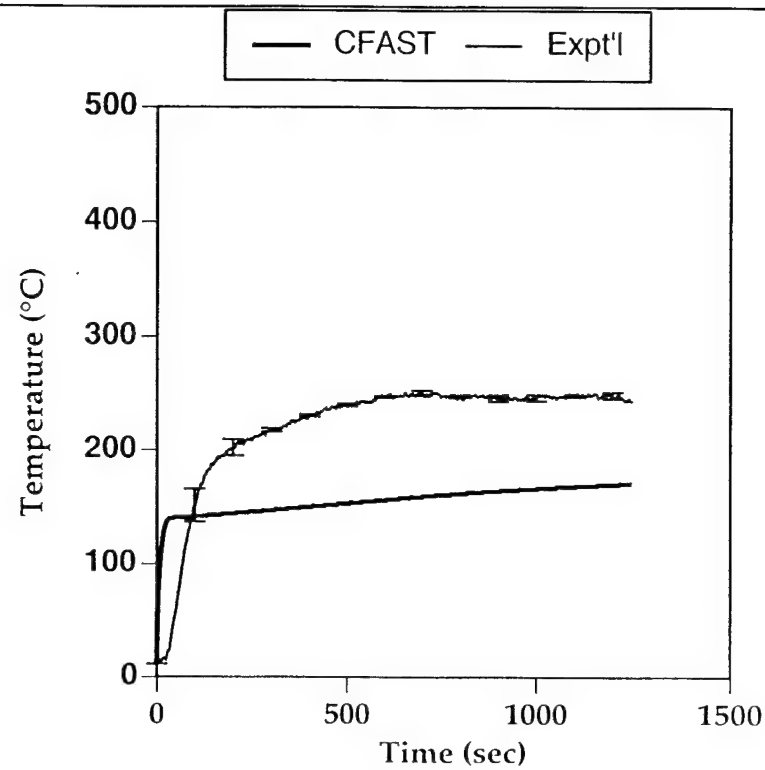

Figure 20A. Predicted versus Measured Laundry Passageway Upper Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

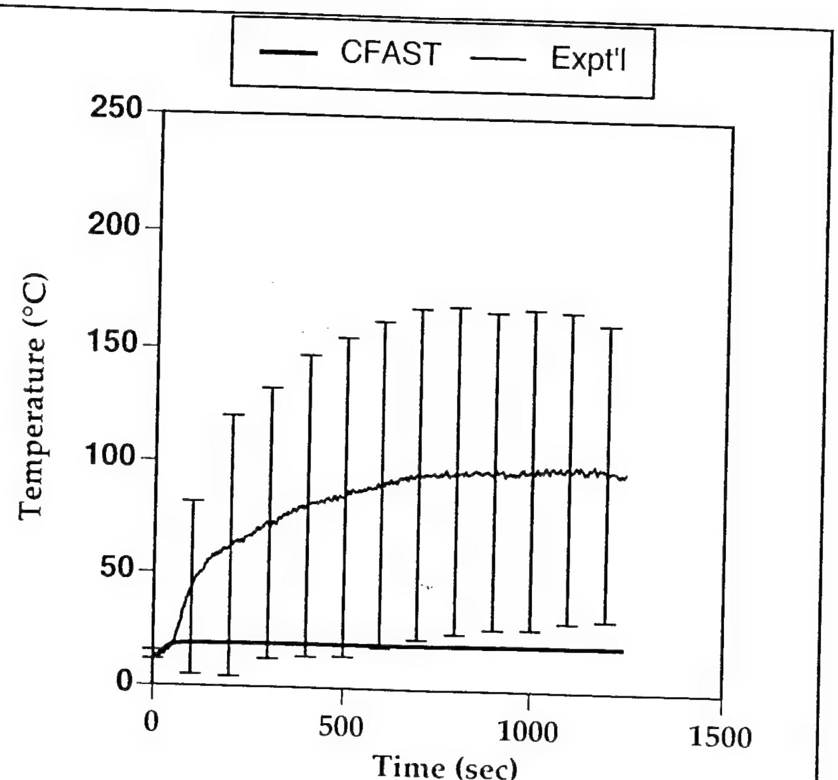

Figure 20B. Predicted versus Measured Laundry Passageway Lower Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

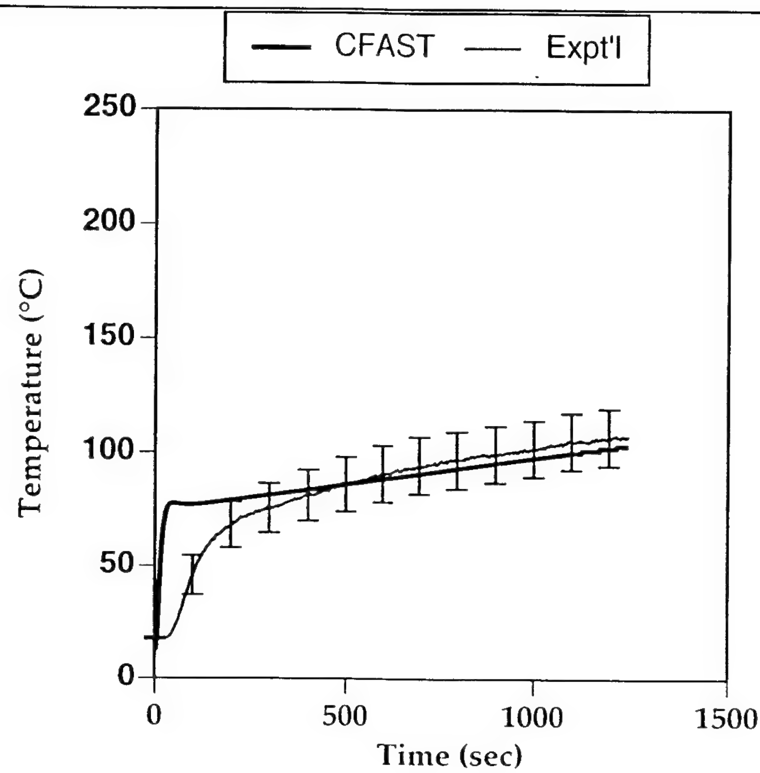

Figure 21A. Predicted versus Measured Wardroom Upper Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

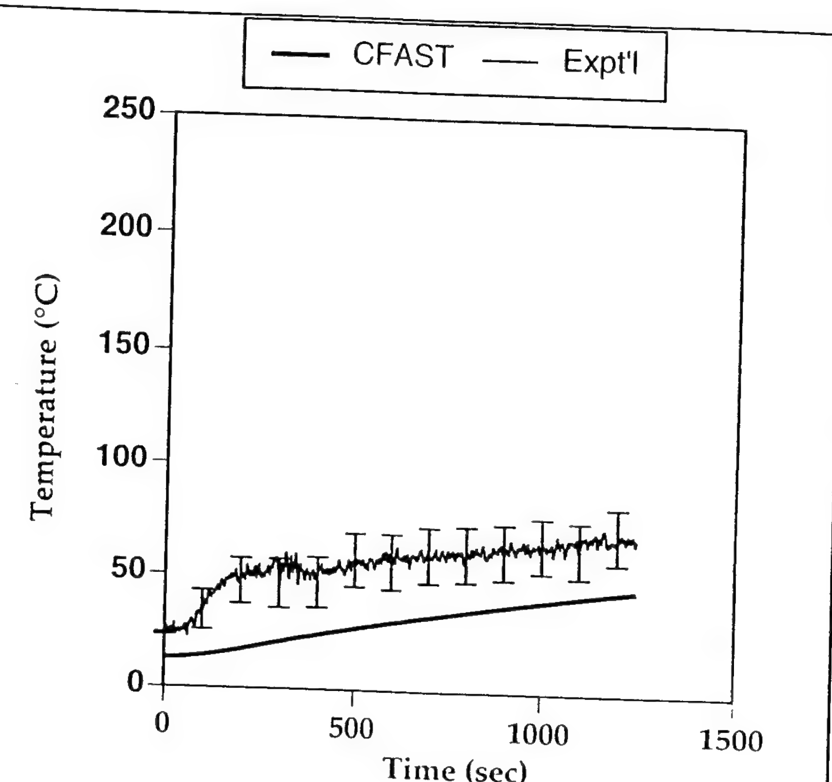

Figure 21B. Predicted versus Measured Wardroom Lower Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

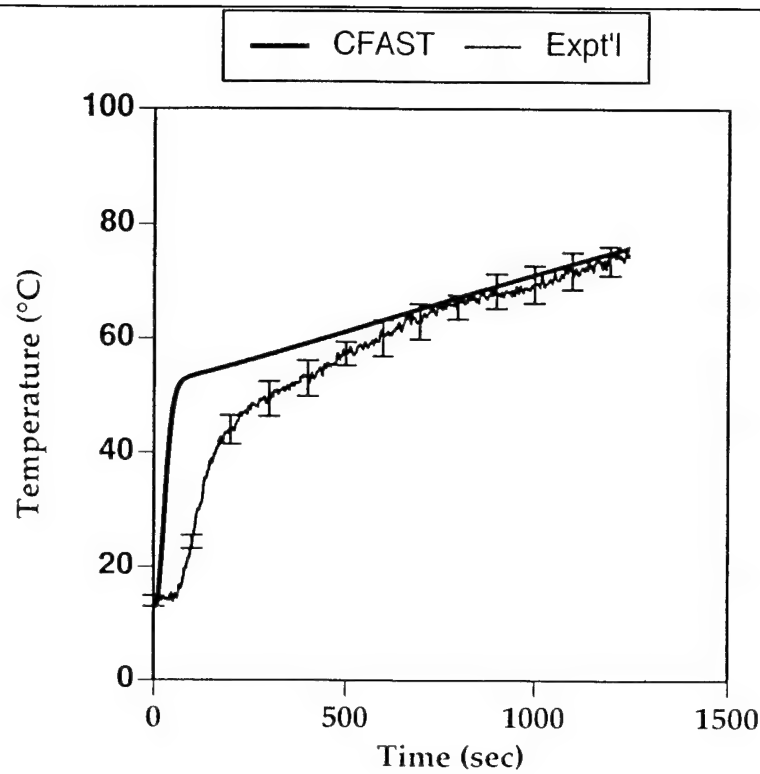

Figure 22A. Predicted versus Measured Navigation Equipment Room Upper Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

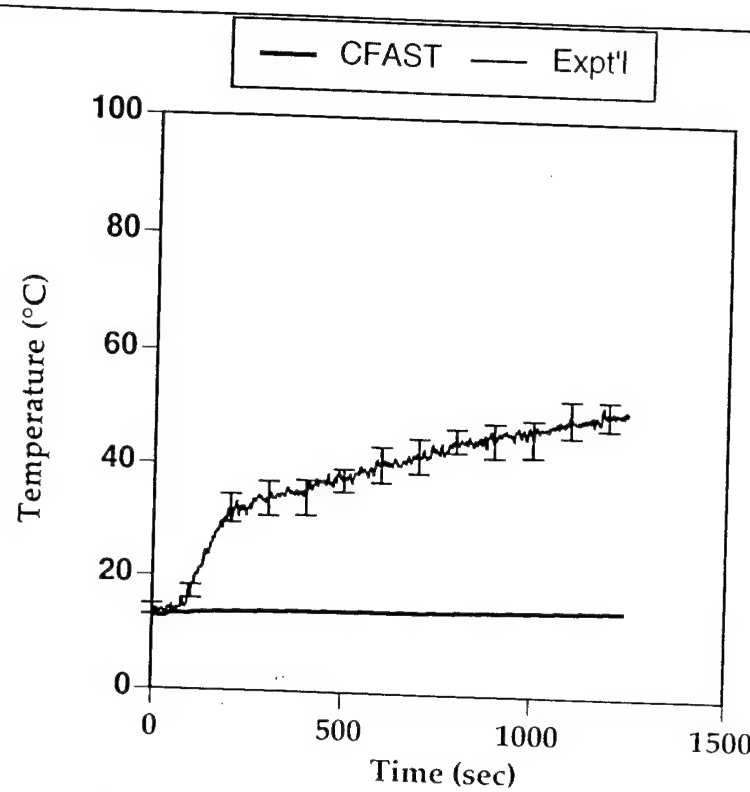

Figure 22B. Predicted versus Measured Navigation Equipment Room Lower Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

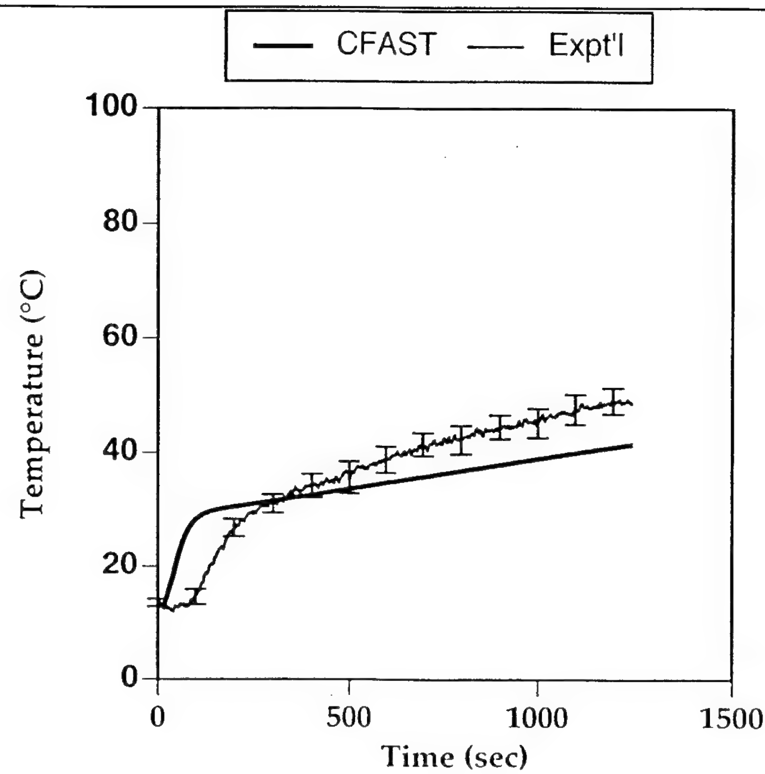

Figure 23A. Predicted versus Measured Control Room Upper Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

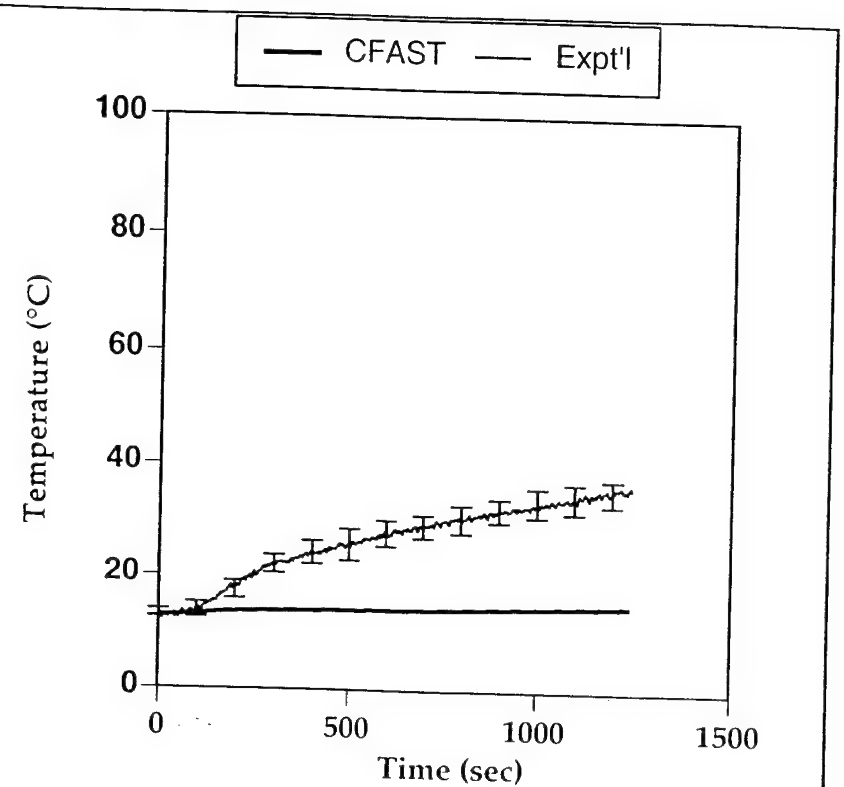

Figure 23B. Predicted versus Measured Control Room Lower Layer Temperatures

The error bars represent one standard deviation in the test data. The Assignment of thermocouples to the upper or lower layer was based on the interface height estimated by CFAST.

There is reasonable agreement between model and test for the upper layer of the Navigation Equipment Room but, given the major discrepancy in the upper layer temperatures for the Wardroom, this result may be coincidental. The observation that the predicted lower layer Navigation Equipment Room temperatures are only slightly higher than the pre-fire temperatures supports this conclusion. Clearly, a column of superheated gas (from the upper layer of the Wardroom) could not rise through the lower layer of the Navigation Equipment Room without heating the latter. The situation in the Control Room is similar — there is no significant increase in the predicted lower layer temperature, resulting in very poor agreement with experiment, but the agreement with the data for the upper layer is surprisingly good.

5.0 EXAMPLES OF ALTERNATIVE INPUTS

In the two previous sections, we outlined an approach to building the "best" model of a specific test case (*i.e.*, one based on the most accurate available inputs). In the process, we have seen several areas in which alternative sets of inputs were possible and in which the decision as to which set should be used was somewhat arbitrary. In this section, we will discuss the results obtained when some of those alternatives are used. Our purpose is to illustrate the general magnitudes of the effects that might be expected.

5.1 Fire Specification Alternatives

In the course of developing the fire specification, we were able to estimate values for the fuel parameters based on *a priori* knowledge regarding the type of fuel. However, we were not able to do the same for the pyrolysis and combustion parameters because they are dependent on the dynamics of the burning process. Typically, the user would make "best guess" estimates of the nominal values for these parameters and then bracket those with high and low extremes. In this section, we provide examples of the effects of some of the key pyrolysis and combustion parameters.

5.1.1 Heat release rate parameters

Equation 1 showed the relationship among ΔH_c, FMASS and FQDOT, the three parameters relevant to heat release rate. In our case study, we specified the first two of these and CFAST calculated the third. That approach was chosen primarily for convenience (FMASS was available from the test data and ΔH_c was known from the type of fuel). It would have been equally valid, although not as convenient, to use either of the other permutations.

Regardless of the manner in which it is defined, the heat release rate is one of the most critical inputs for CFAST. Accordingly, it is appropriate that we consider the effects of changing this value. Due to the way in which our problem was originally set up, the easiest way to effect this change was to adjust the mass loss rates (FMASS) and allow CFAST to calculate new values for FQDOT.

For our comparison, the Laundry Room model was run with one half, two times and three times the nominal heat release rates. Figures 24A and 24B shows the effects of these changes on the upper and lower layer air temperatures, respectively. As may be readily seen, there are significant effects on the qualitative behavior of the predictions as well as on the quantitative results. We should note that the nominal pyrolysis rate was about 24 grams per second, so the results shown here correspond to changes in pyrolysis rate of only a few grams per second.

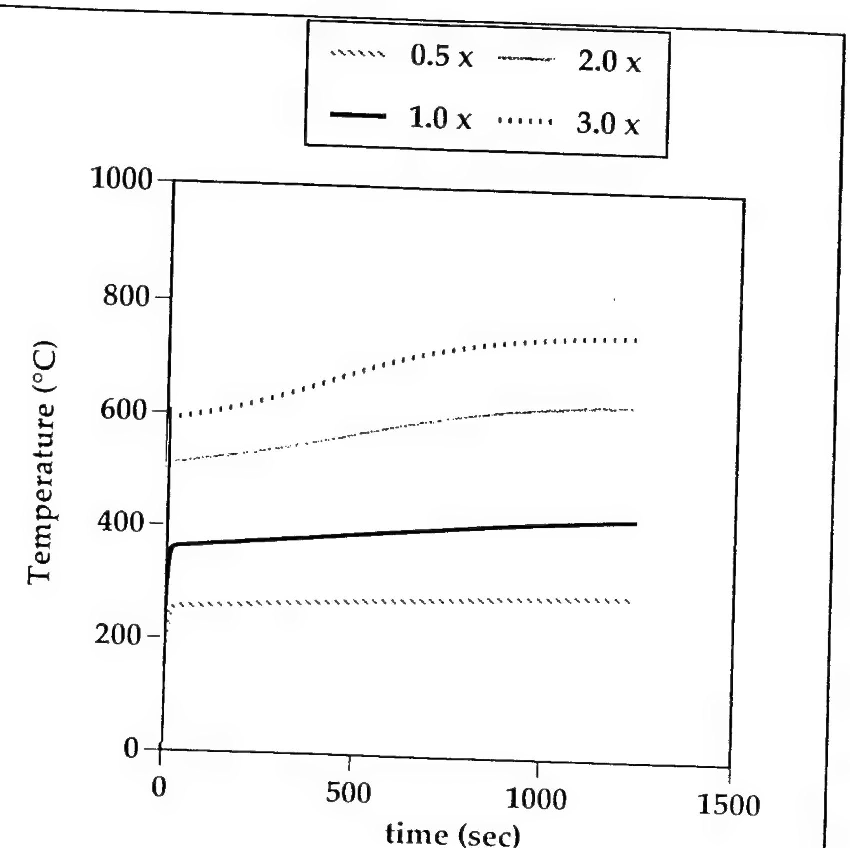

Figure 24A. Effect of Heat Release Rate on Laundry Room Upper Layer Temperatures

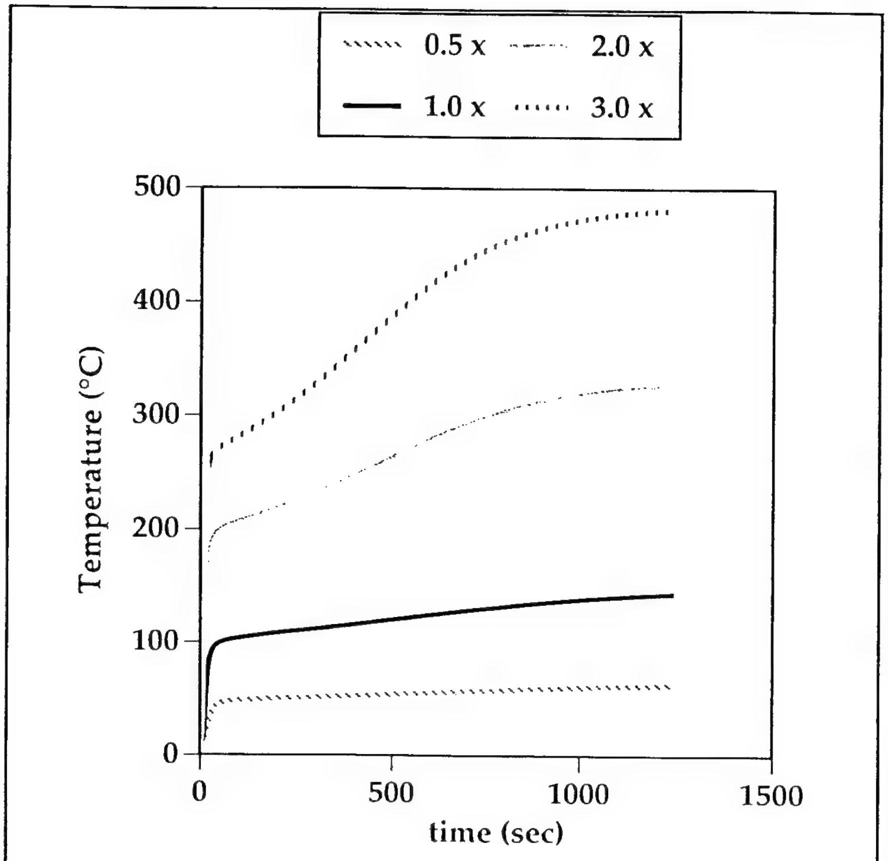

Figure 24B. Effect of Heat Release Rate on Laundry Room Lower Layer Temperatures

5.1.2 The OD parameter

As was discussed above, OD specifies the mass ratio of soot to carbon dioxide in the combustion products. Clearly, this will affect the predicted soot concentrations. Perhaps less obviously, it will also affect temperatures (because soot is an important factor in radiation transport) and concentrations of carbon dioxide and carbon monoxide (because carbon which appears as soot is unavailable for production of other carbon-containing species). To illustrate these effects, we ran the Laundry Room model using OD values of 0.00, 0.06 and 0.10. All other inputs were set to their nominal values, as given in Listing 5.

Figure 25 shows the predicted soot concentrations for the Laundry Room. As might be expected, the soot concentrations are approximately linear with OD[24] and no soot is produced when OD is zero. It is important to note that zero is the default OD input and, therefore, if the user fails to specify a different value, CFAST will predict no soot formation. As we will see in the following paragraphs, this is likely to result in major errors in the temperature predictions.

The effects on upper and lower layer air temperatures may be seen in Figure 26. In the upper layer, the temperature is much higher when there is no soot (OD = 0.00) than when there is soot. However, there is a negligible difference between OD values of 0.06 and 0.10. The temperature reduction that occurs when soot is present is caused by the high emissivity of soot particles which, if present, cool the upper layer very efficiently. The similarity of the temperatures for the two cases in which soot is present is due to a saturation effect. At low concentrations, photons emitted from each soot particle easily escape from the layer but, at some soot concentration, the particle density becomes high enough that most photons are absorbed and emitted several times before escaping. Increasing the amount of soot beyond this point has little additional effect.

The effects on lower layer temperature differ from the above in two respects. First, the soot concentrations are low enough that we do not see saturation. More importantly, high soot concentrations in the lower layer lead to higher, rather than lower, air temperatures. This is due to the fact that the upper layer of the fire compartment is directly heated by mass injection from the fire plume while the lower layer is not. As a result, the upper layer is much hotter than the surroundings, leading to a net loss of energy by radiation. In the lower layer, which is cooler than the adjacent upper layer, there is a net absorption.

Carbon monoxide and dioxide concentrations for the Laundry Room are illustrated in Figure 27 and 28. Although the absolute concentrations of these two species are very different, the trends with respect to OD are similar. In the upper layer, where the effects of altering the species production factors are seen directly, the concentrations of both species are inversely correlated with OD. As mentioned above, this is due to increasing sequestration of carbon in the form of soot, leaving less carbon available for any other species, as OD increases.

[24] Note that this (approximate) linearity applies only to changes in the OD value within a given model. There is no general relationship between soot concentrations for different models (those that differ in regard to parameters other than OD).

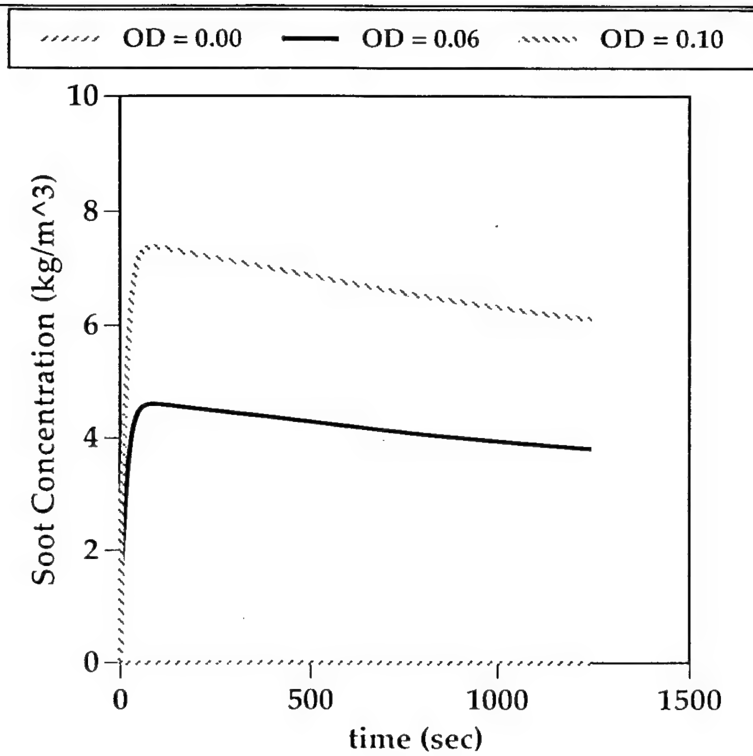

Figure 25A. Effect of OD Parameter on Laundry Room Upper Layer Soot Concentrations

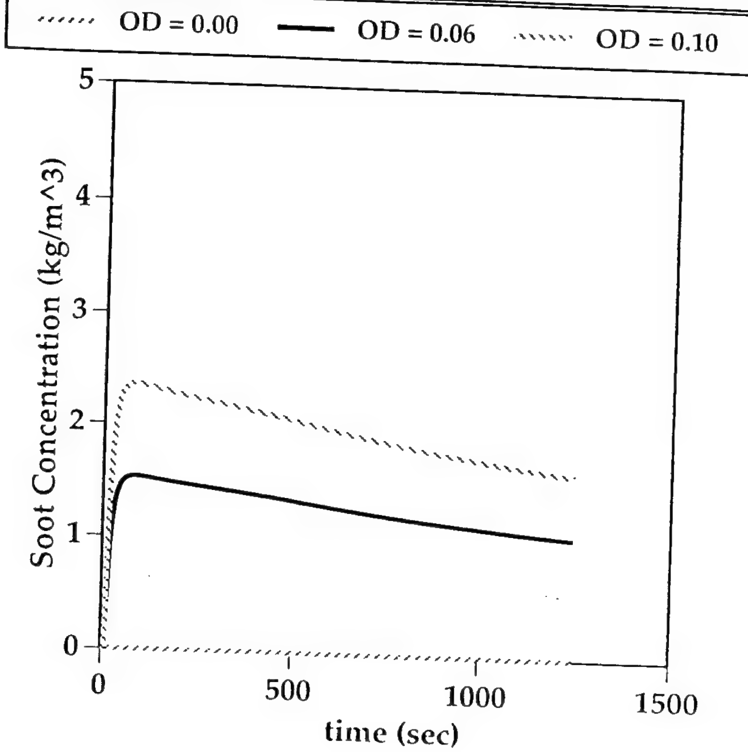

Figure 25B. Effect of OD Parameter on Laundry Room Lower Layer Soot Concentrations

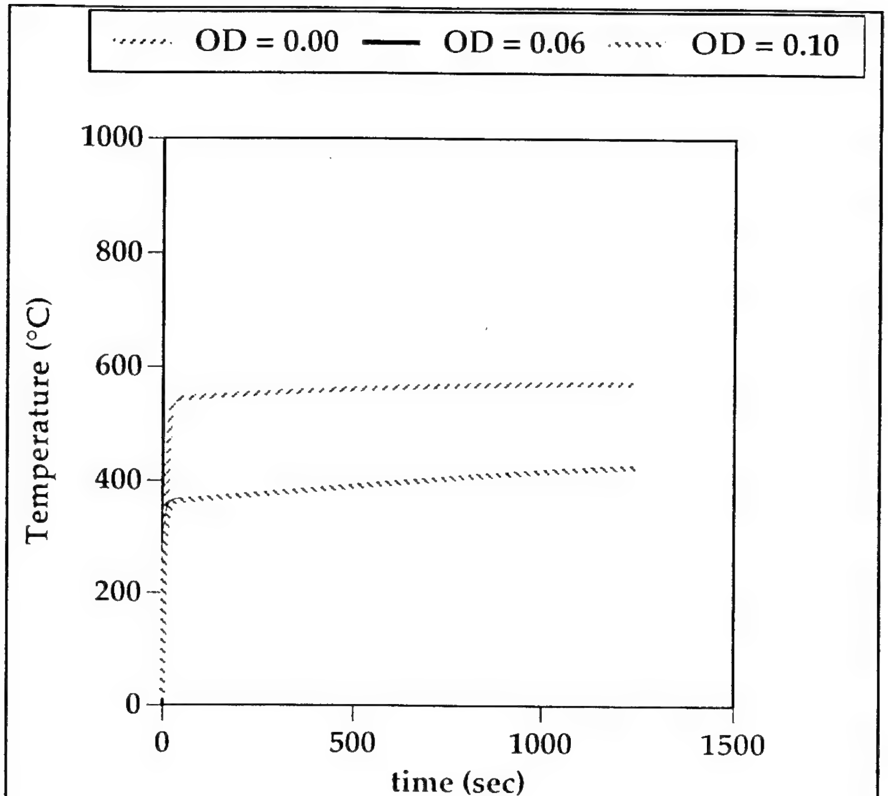

Figure 26A. Effect of OD Parameter on Laundry Room Upper Layer Temperatures

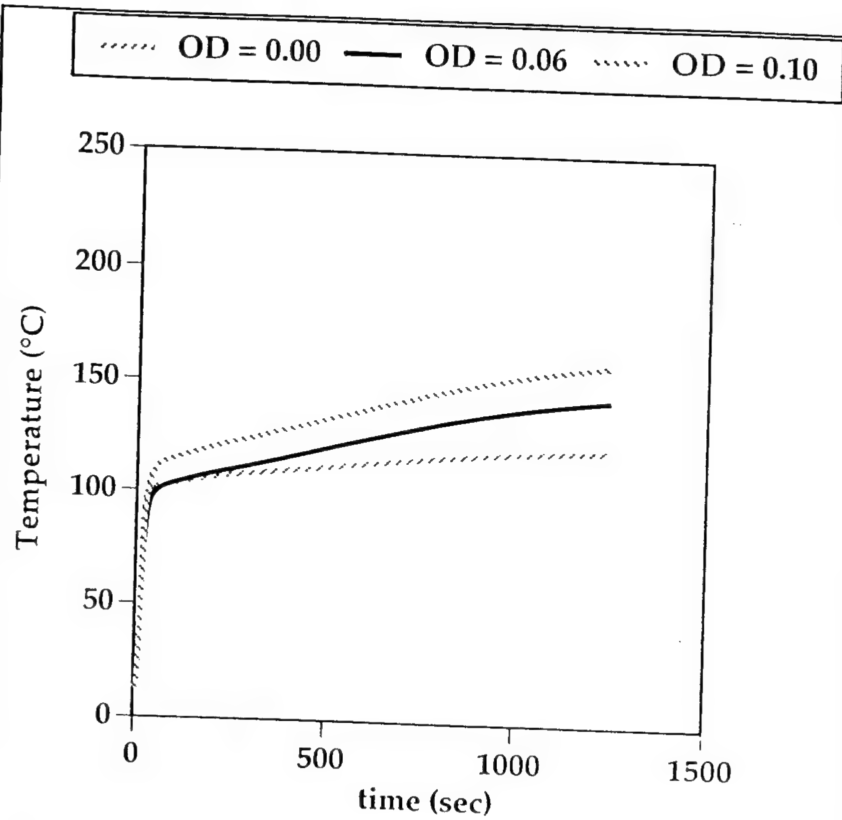

Figure 26B. Effect of OD Parameter on Laundry Room Lower Layer Temperatures

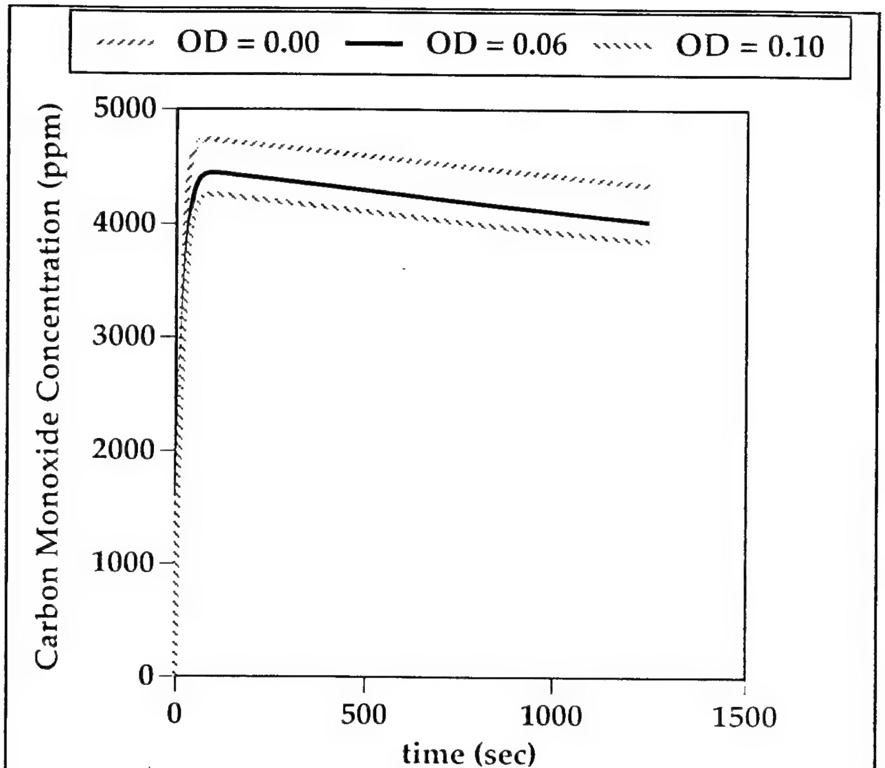

Figure 27A. Effect of OD Parameter on Laundry Room Upper Layer Carbon Monoxide Concentrations

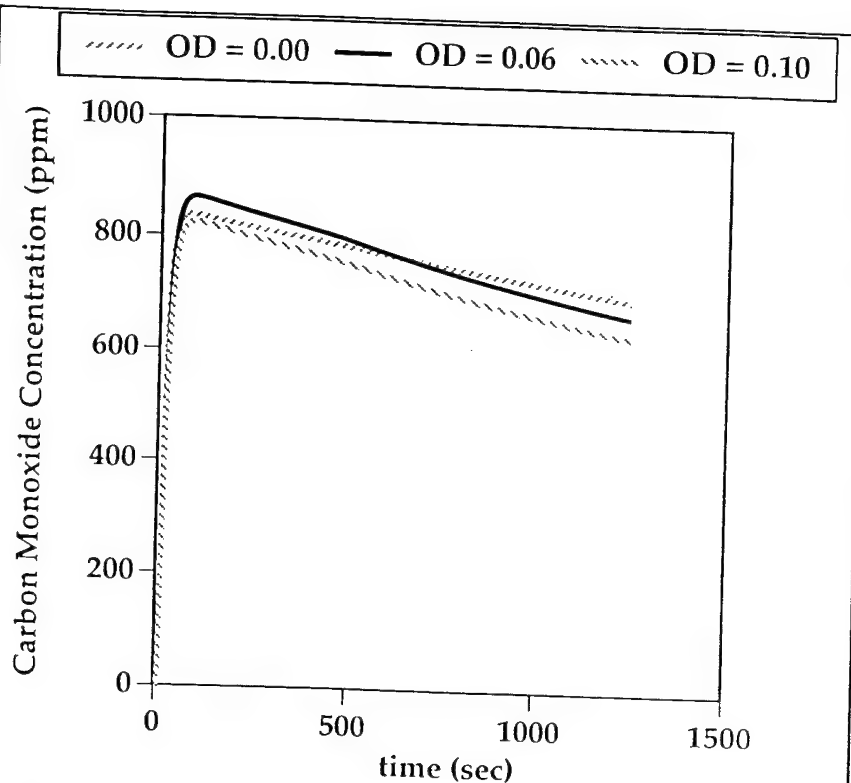

Figure 27B. Effect of OD Parameter on Laundry Room Lower Layer Carbon Monoxide Concentrations

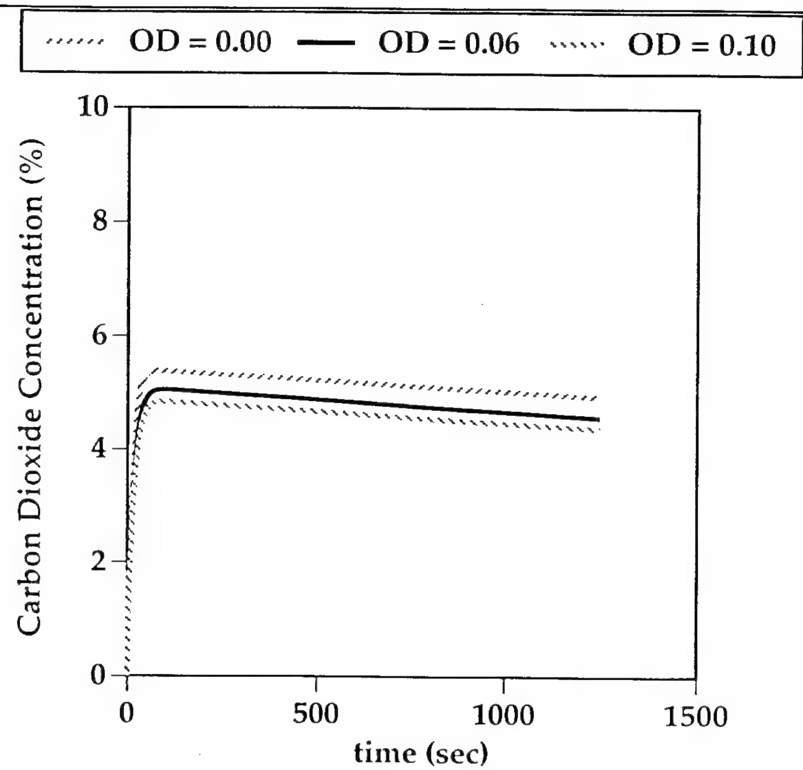

Figure 28A. Effect of OD Parameter on Laundry Room Upper Layer Carbon Dioxide Concentrations

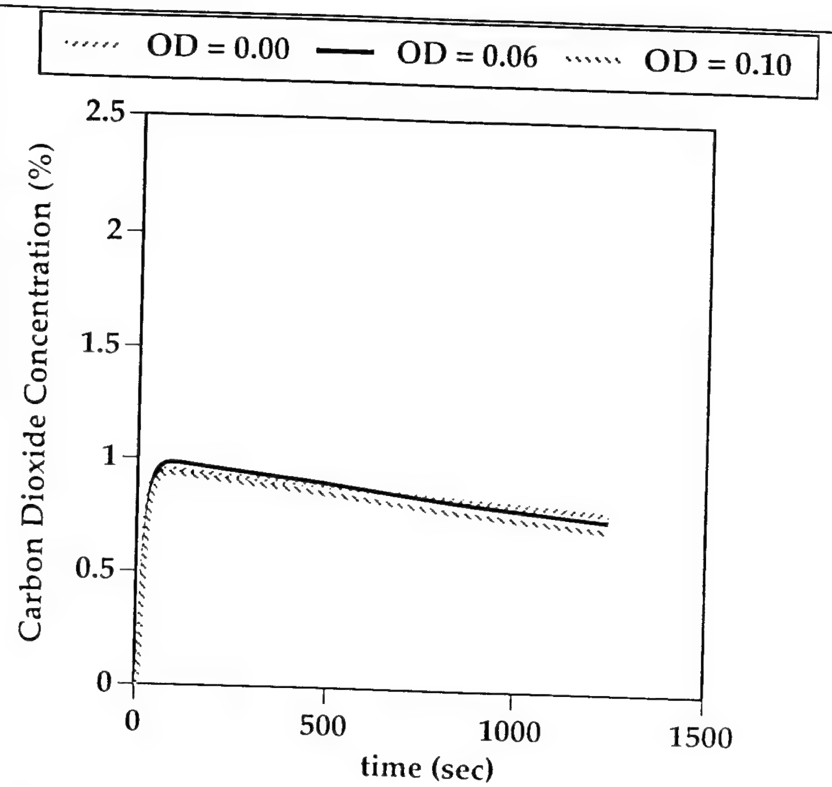

Figure 28B. Effect of OD Parameter on Laundry Room Lower Layer Carbon Dioxide Concentrations

For the lower layer, the effects of changes in the species production ratios are confounded by other factors. In particular, lower layer concentrations depend on mixing effects which, in CFAST, occur in the horizontal vents where there are opposing jets of hot and cold air entering and exiting the compartment. Since vent flows are affected by temperature, pressure and layer heights, the lower layer concentrations are complex functions.

5.1.3 The CO parameter

Figure 29 shows that carbon monoxide concentrations are approximately linear with respect to CO in the same way that soot is approximately linear with OD. Like OD, the CO input has a large effect only of the species which it directly controls and relatively small indirect effects on concentrations of other carbon-containing species (Figures 30 and 31). However, the CO parameter has almost no effect on layer temperatures, as shown in Figure 32. The practical implication of this is that, unless predicting carbon monoxide concentration is an important goal of the simulation, the value used for the CO input is rather unimportant. This is fortunate, because CO is one of the most difficult parameters to specify *a priori*.

5.2 Geometry Specification Alternatives

The primary reason for the decision to use a compartment rearrangement, rather than a virtual compartment, approach was our observation that, with virtual compartments, the Laundry Passageway vertical vent had to be eliminated from the model in order for the simulation to run to completion. Using the rearrangement method, that vent could be included (although it did have to be reduced in size). We later found that the addition of the Wardroom lifted this vent size restriction.

In this section, we develop the "dummy" compartment concept as a possible method for circumventing the vertical vent problems. We also illustrate the use of virtual compartments and revisit the vertical vent area issue. Although not all of these methods were used in our case study, we believe that they may be applicable to other simulation problems.

5.2.1 Dummy compartments

Recall that the virtual compartment method involved treating a single real compartment as if it were two (or more) "virtual" compartments (see Figure 13). The "dummy" compartment concept differs from this in that we proposed to add to the model a new compartment that had no counterpart in reality.

The rationale for this is as follows:

1. We have observed that stalling problems frequently are associated with the furthest downstream vertical vent (*i.e.*, one that connects to the exterior), therefore it is possible that replacing the exterior with a dummy compartment (so that the vent in question no longer connects to the exterior) might alleviate the problem.

2. We know that the effects of adding a new compartment propagate upstream (back toward the fire compartment) so that the predictions for pre-existing compartments can be altered by the addition.

3. We hypothesized that, if the new compartment was large enough and had a sufficiently low flow resistance with respect to the exterior, the new compartment would be transparent to CFAST (*i.e.*, the model predictions would be the same as if the compartment did not exist). We called a compartment meeting these criteria a "dummy" compartment.

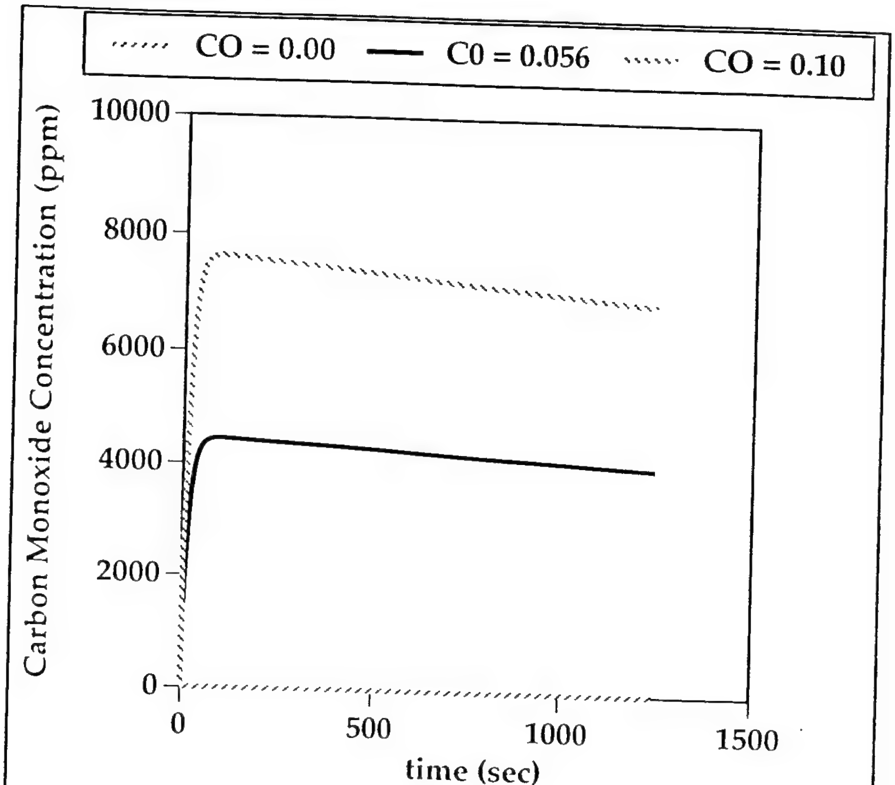

Figure 29A. Effect of CO Parameter on Laundry Room Upper Layer Carbon Monoxide Concentrations

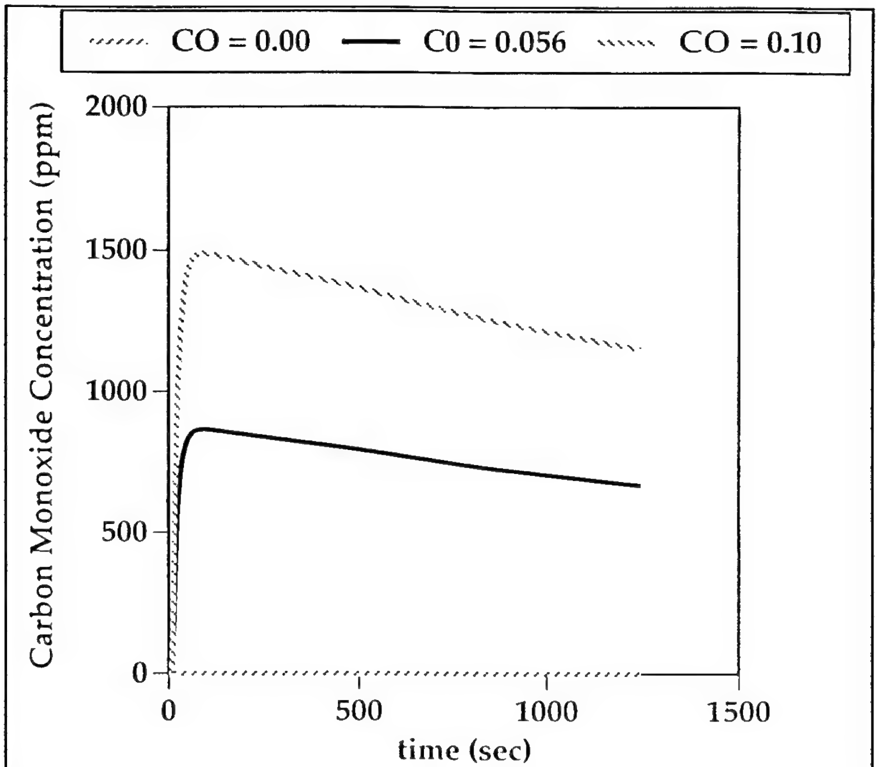

Figure 29B. Effect of CO Parameter on Laundry Room Lower Layer Carbon Monoxide Concentrations

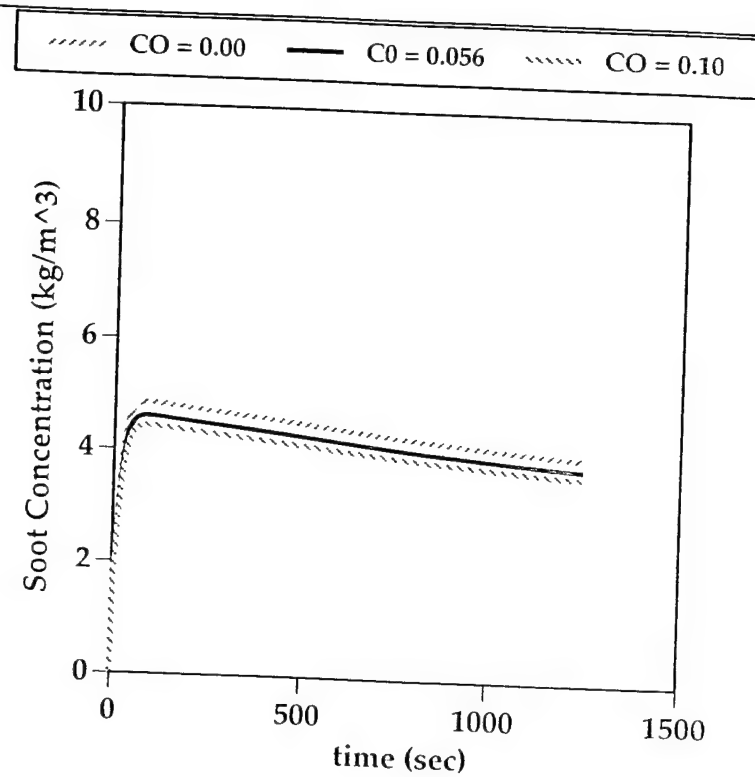

Figure 30A. Effect of CO Parameter on Laundry Room Upper Layer Soot Concentrations

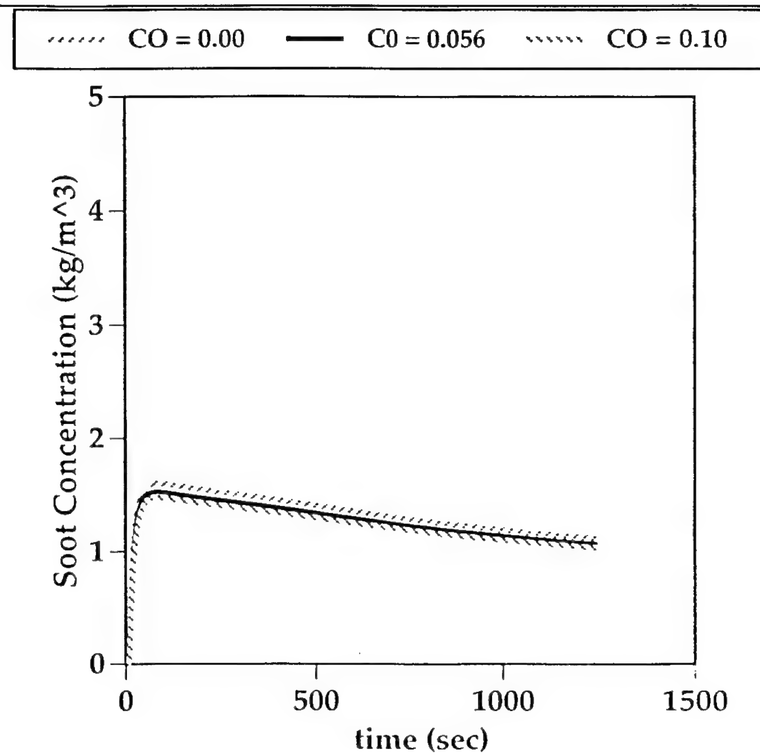

Figure 30B. Effect of CO Parameter on Laundry Room Lower Layer Soot Concentrations

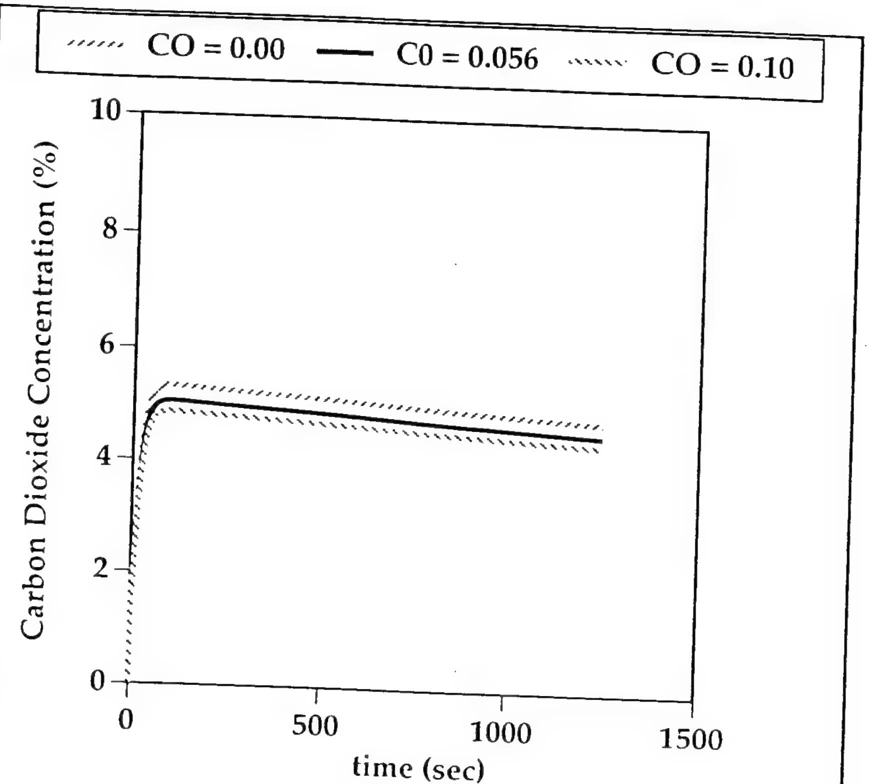

Figure 31A. Effect of CO Parameter on Laundry Room Upper Layer Carbon Dioxide Concentrations

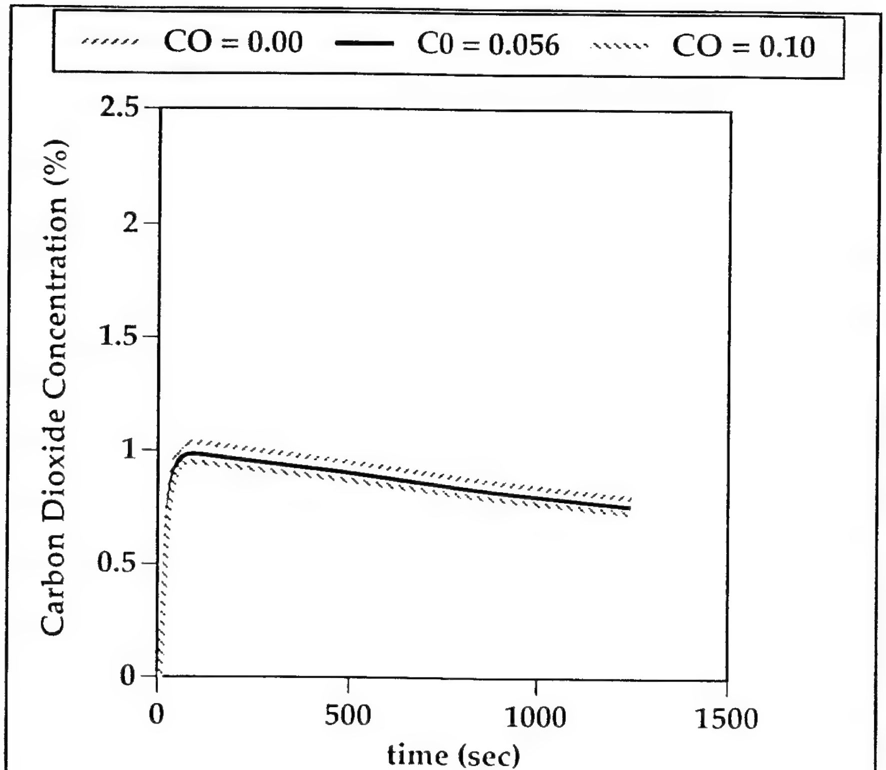

Figure 31B. Effect of CO Parameter on Laundry Room Lower Layer Carbon Dioxide Concentrations

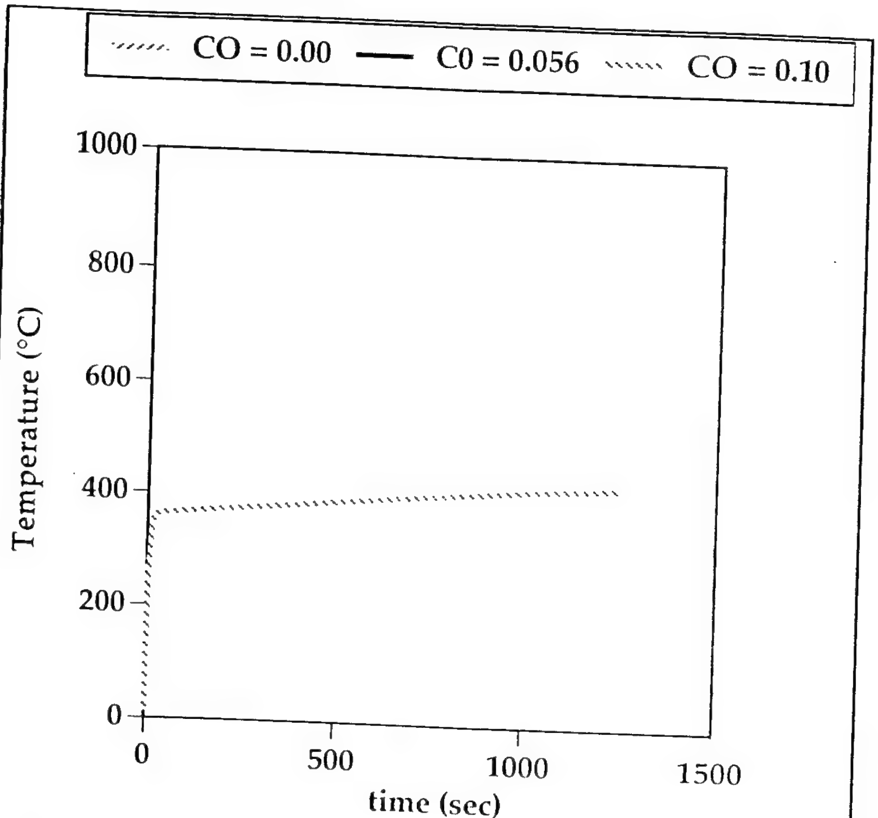

Figure 32A. Effect of CO Parameter on Laundry Room Upper Layer Temperatures

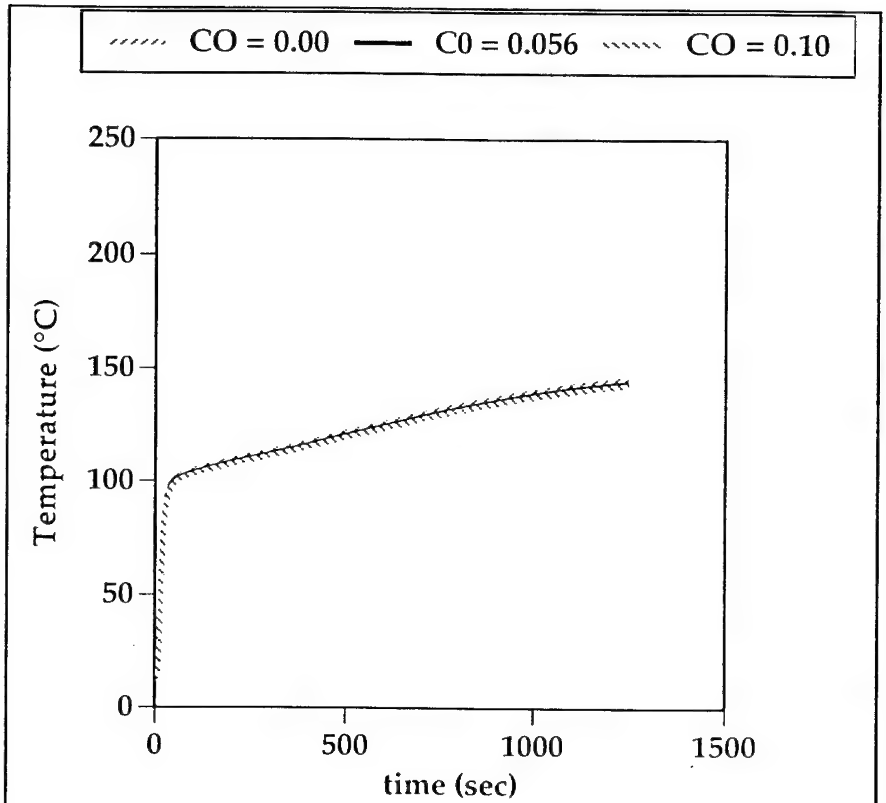

Figure 32B. Effect of CO Parameter on Laundry Room Lower Layer Temperatures

To test this hypothesis, we went back to the rearranged compartment version of the Laundry Passageway and added a new compartment connected to the Laundry Passageway via the vertical vent. Since we had no guidance regarding the minimum size appropriate for a dummy compartment, we tried 10, 100 and 1000 meter (33, 328 and 3281 ft) cubes, each of which had an open face [areas of 10^2, 10^4 and 10^6 m^2 (approximately 10^3, 10^5 and 10^7 ft^2) respectively]. For comparison with our prior work, the vertical vent (from the Laundry Passageway to the dummy compartment) was set to an area of 0.25 m^2 (2.69 ft^2) in all three models.

The Laundry Passageway temperature predictions for these models are compared with the previous results in Figure 33. We see that the predicted temperatures for the cases in which a dummy compartment was used always differed from those where there was no dummy compartment. For the upper layer, the volume of the dummy compartment had a negligible effect; in the lower layer, the compartment volume did have an effect, but only for the 10^9 m^3 (35 x 10^9 ft^3) case. Figure 34 shows that, for the Laundry Room, the dummy compartment method predicts air temperatures very similar to those obtained without the dummy compartment.

The dummy compartment hypothesis is not supported by these results – even when the volume of the dummy compartment is exceedingly large, the existence of the compartment does effect the rest of the model. However, those effects appear to be most serious for the compartment directly connected to the dummy and may be relatively small, even negligible, in the vicinity of the fire. This suggests that the concept may be a useful approximation in some circumstances as long as the dummy compartment volume is not excessive. Clearly, the technique will introduce some inaccuracies, especially for the compartments immediately upstream of the dummy, but those errors must be compared with the errors that would be caused by the use of an incorrect vertical vent area.

5.2.2 Virtual compartments

In order to demonstrate the application of virtual compartments and the combination of virtual and dummy compartments, we again focused on the Laundry Passageway. The previously developed input files for the that compartment (Listings 6 and 7) were modified by addition of a dummy compartment (with the same dimensions as the Wardroom[25]) having a door to the exterior [equivalent to the entire 8.51 m (27.92 ft) x 2.59 m (8.50 ft) Wardroom bulkhead]. These changes permitted the Laundry Passageway vertical vent to be increased to the correct area [0.78 m^2 (8.40 ft^2)] without stalling the simulation. We should note that, as discussed above, these results are expected to be different than those that would have been obtained in the absence of the dummy compartment. Unfortunately, due to the vent area problem, the latter case could not be simulated.

In the absence of a bulkhead between the virtual compartments, we might expect that the two upper layers would be mixed to produce a constant temperature zone and that the same would be true of the lower layers. However, this is not the case – CFAST calculates conditions for each of the four zones independently, resulting in discontinuities at the boundary between the two virtual compartments. This is most evident in the upper layer temperatures, which differ by about 50°C (Figure 35A). Note that the two values bracket the value that was obtained when the Laundry Passageway was treated as a single compartment. Results for the virtual compartment lower layers (Figure 35B) also bracket the those of the single-compartment passageway model, but the differences among the three predictions were negligible in this case.

[25] We also performed sensitivity tests to verify that the results with this volume (approximately 88 m^3) were the same as those obtained with very large dummy compartments (in excess of 10^3 m^3).

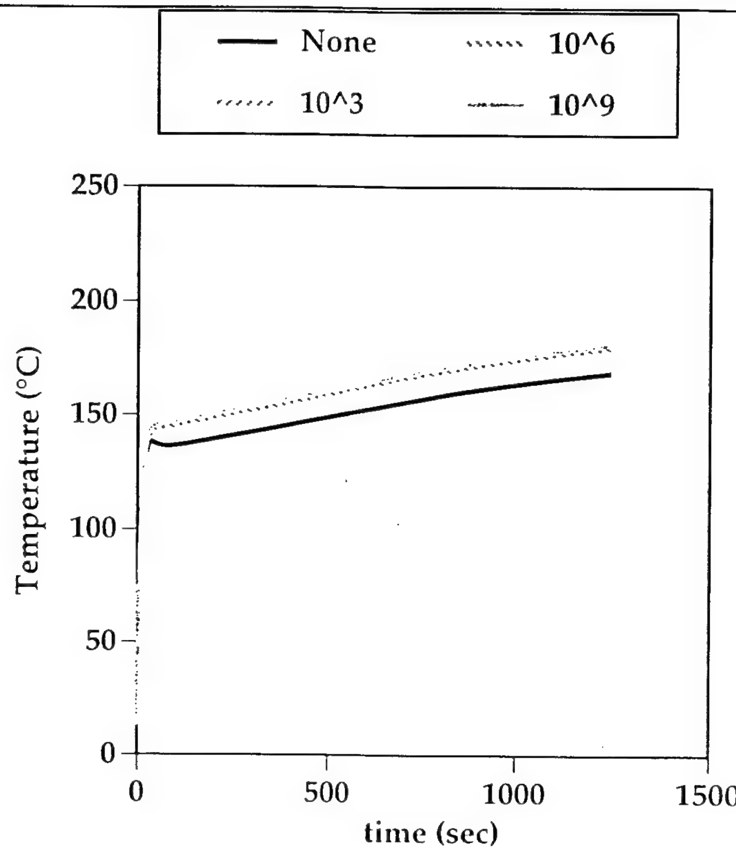

Figure 33A. Effect of Dummy Compartment on Laundry Passageway Upper Layer Temperatures

The presence of a dummy compartment changed the model predictions for the Laundry Passageway upper layer but there was negligible dependence on the dummy compartment volume over the range 10^3 to 10^9 m^3 (35×10^3 to 35×10^9 ft^3).

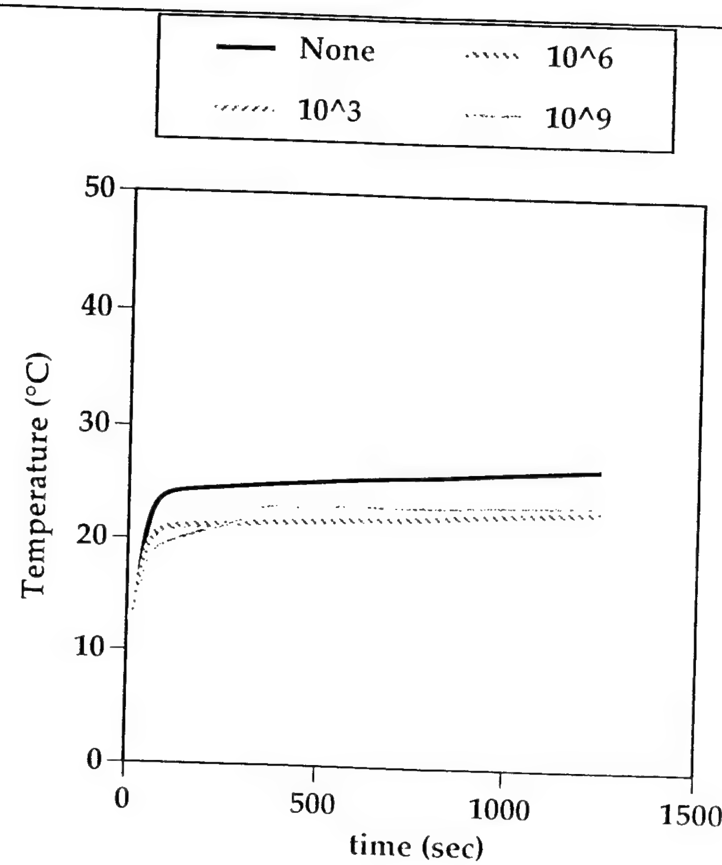

Figure 33B. Effect of Dummy Compartment on Laundry Passageway Lower Layer Temperatures

The presence of a dummy compartment changed the model predictions for the Laundry Passageway lower layer. The was no dependence on dummy compartment volume below 10^6 m^3 (35×10^6 ft^3)., but there were effects at the largest volume.

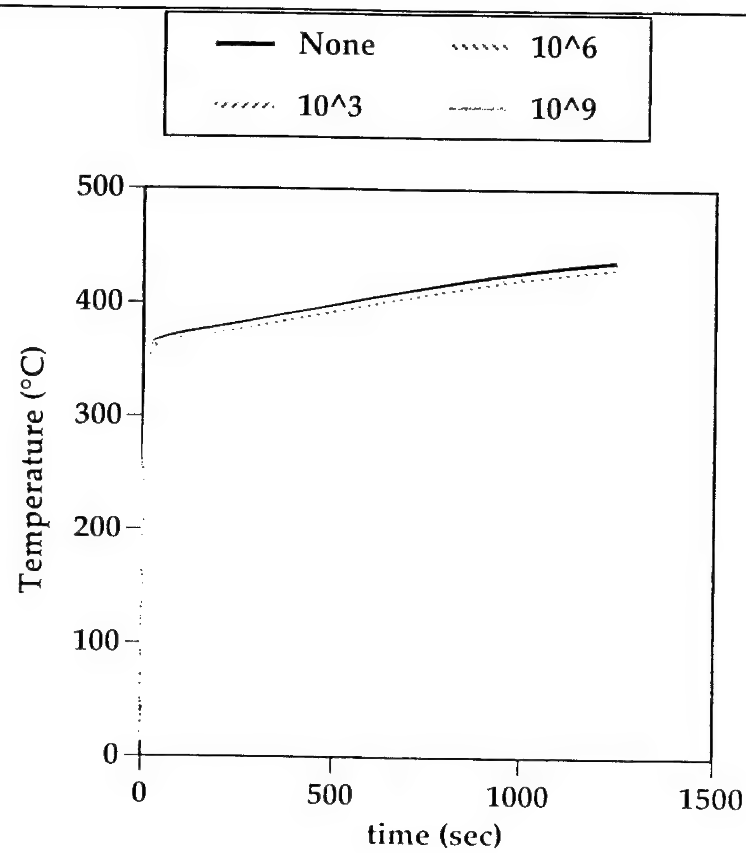

Figure 34A. Effect of Dummy Compartment on Laundry Room Upper Layer Temperatures

The presence of a dummy compartment had an almost undetectable effect on the Laundry Room upper layer temperature predictions.

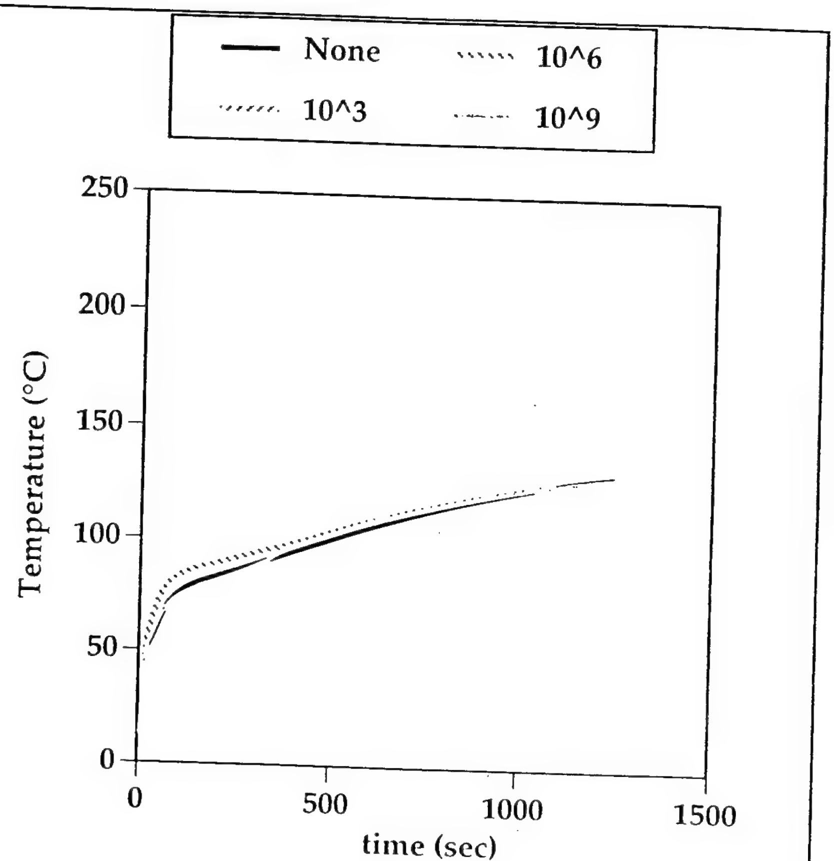

Figure 34B. Effect of Dummy Compartment on Laundry Room Lower Layer Temperatures

The presence of a dummy compartment a small but detectable effect on the Laundry Room lower layer temperature predictions, especially for the largest volume.

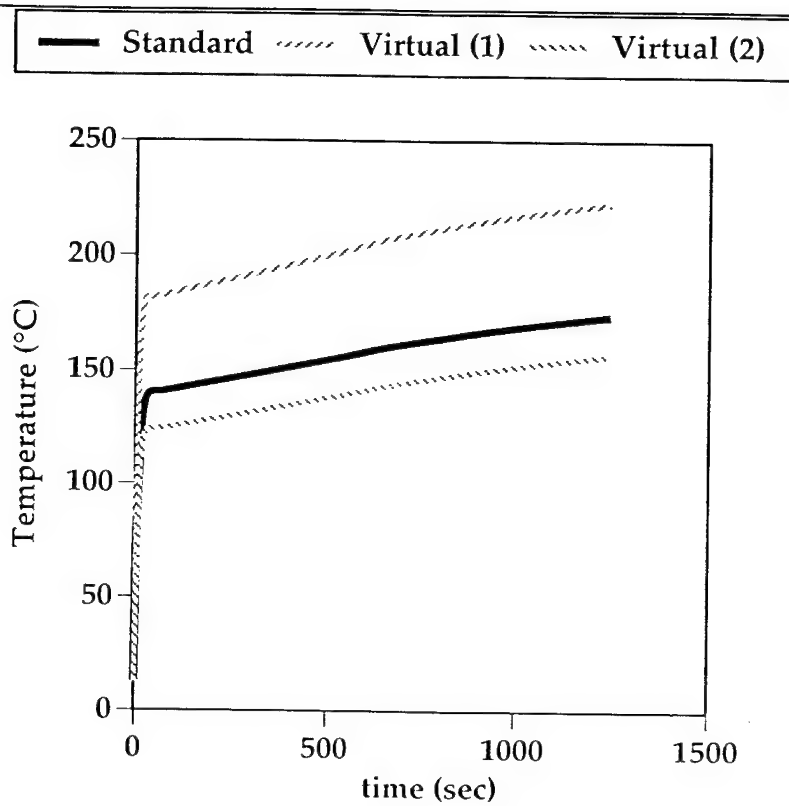

Figure 35A. Effect of Virtual Compartments on Laundry Passageway Upper Layer Temperatures

Temperatures of the two virtual compartments that, collectively, represented the Laundry Passageway were different from each other and from those predicted when the passageway was treated as a single compartment.

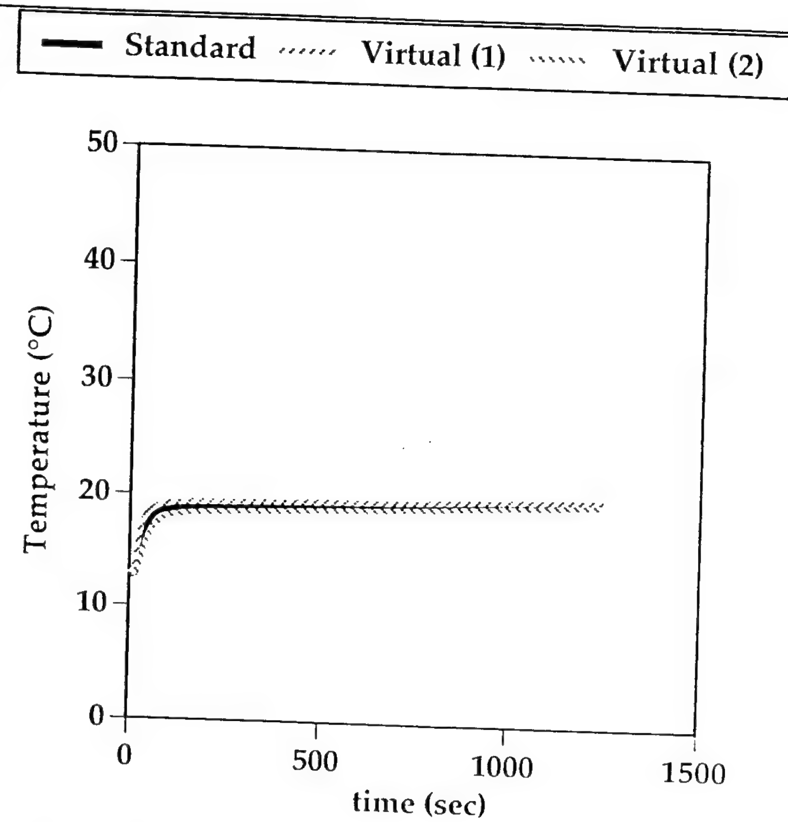

Figure 35B. Effect of Virtual Compartments on Laundry Passageway Lower Layer Temperatures

For the lower layer, the temperatures of the two virtual compartments that, collectively, represented the Laundry Passageway were essentially the same and agreed with those predicted when the passageway was treated as a single compartment.

5.2.3 Vertical vent size

As a result of our experiences, it became obvious that some compromises would often be necessary in models involving vertical vents. We have shown that there are methods, such as dummy compartments, that may permit correctly sized vents to be included, but those techniques introduce their own errors. Clearly, the user will have to make a trade-off and, to do that, will need some idea of the relative magnitude of the errors of the different techniques. In a preceding section, we presented information regarding the inaccuracies of the dummy compartment approach: in this section we consider the effects of altering the vertical vent area.

The impact of vent area was investigated by systematically varying the area from zero to approximately one half of the area of the Laundry Passageway overhead. Temperature predictions for selected vent areas are shown in Figures 36A and 36B. For the upper layer, the air temperatures tended to rise to a maximum in the first minutes, then abruptly drop. With very small and very large vents, a quasi-equilibrium state was reached in which the temperatures increased slowly for the remainder of the simulation. The peak and quasi-equilibrium temperatures decreased as the vent area was increased. Venting of the hottest gases via the opening in the overhead would be expected to lower the air temperature, so the inverse dependence of upper layer temperature on vent area is in agreement with intuition.

In the lower layer, the situation was more complicated. For the smallest vent, the temperatures simply leveled off with no peak; for the largest vent, there was a pronounced peak and a large subsequent drop. The data are inconclusive for the intermediate cases due to the stalls which occurred before the peak temperature was reached, but suggest that the temperatures rose faster (and possibly would have reached higher values) for larger vents. A possible explanation for this is that larger overhead vents in the passageway allow a greater flow of hot air from the fire compartment.

As expected, these results show that the area of a vent in the overhead has a significant effect on the temperatures in the compartment, especially in the upper layer. They also show that the magnitude (and even the sign) of this effect is not readily predictable. In the event that the model does not run with the actual vent areas, it may be necessary to substitute a different area. However, if this is done, it is important that the user carefully investigate the effects of that change.

6.0 RECOMMENDATIONS

In the preceding sections, we provided examples of the use of CFAST in modeling a specific problem relevant to the Navy. In this section, we will present some general recommendations for the application of CFAST in other problems.

It is important to start with a clear idea of the goals of the modeling: Are you trying to simulate a specific fire or are you interested in the behavior for a variety of possible fires? What constitutes "good" versus "poor" performance for your model? How important are temperature predictions as compared with species concentration predictions? Is the interest primarily in vertical or horizontal fire spread?

The better, and more narrowly, the problem can be defined, the more likely it is that useful results will be obtained. When you must make trade-offs (and you will be forced to make them in all but the most trivial problems), refer to your statement of the goals when deciding which details may be neglected and which must be kept.

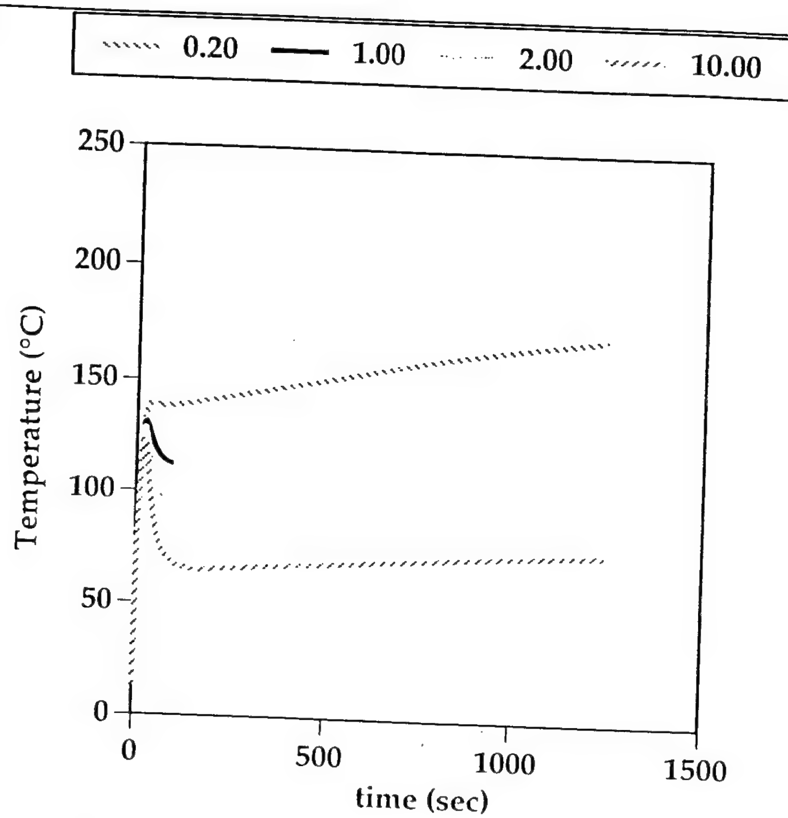

Figure 36A. Effect of Vertical Vent Area on Laundry Passageway Upper Layer Temperatures

The upper layer temperature trends appear to be inversely related to the vent area (in m^2) but the amount of data is limited because the model failed to run to completion for a range of vent areas.

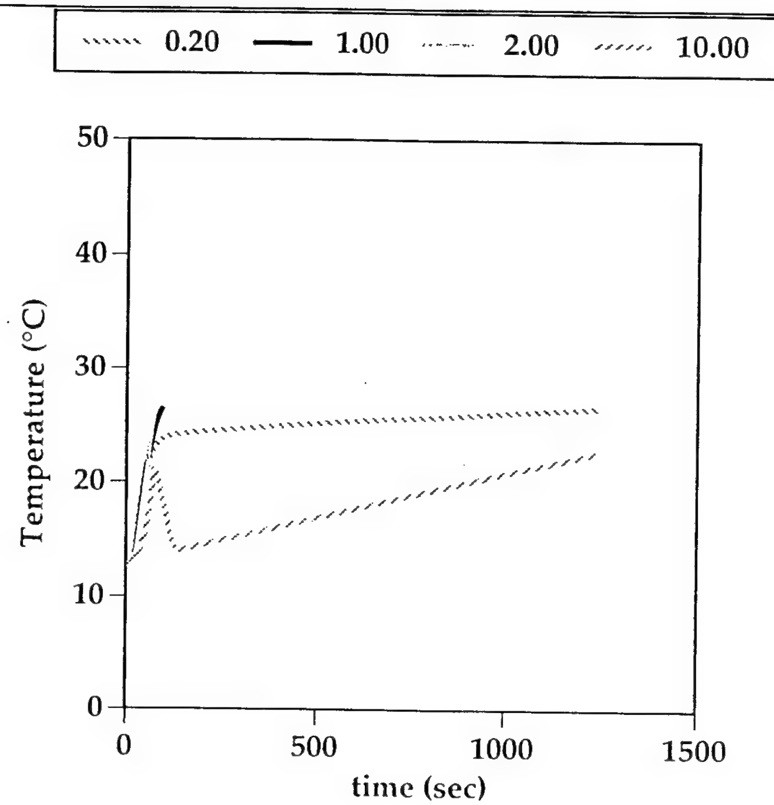

Figure 36B. Effect of Vertical Vent Area on Laundry Passageway Lower Layer Temperatures

The lower layer temperature trends show no clear correlation between the temperature and the vent area (in m²).

For the situation in which a specific fire is to be simulated, it is necessary to collect all of the available information relating to that fire. The process of simulating a specific fire will not be further discussed here because examples were provided as part of our case study. For the more typical case, in which the general performance under a variety of fire conditions is of interest, the use of a Monte Carlo approach is suggested. With that method, the expected performance of various ship designs could be compared, using a statistical analysis of the model predictions, and the results of that analysis could be presented in terms of the probabilities of various outcomes, given a specified range of inputs. For example, modeling one design for a berthing space might indicate that, for fires in the 100 - 250 kW range, there is a 50% probability that the entire space would become uninhabitable within the first two minutes whereas, for a competing design, the probability might be only 25%.

To conduct this type of analysis, the minimum and maximum realistic fire loads would first be estimated based on the expected contents of the compartment. A series of fires, covering the entire range of fire sizes, would then be simulated at a variety of locations. Possible fires should initially be described in general terms: What are the fire classifications? What is the range of anticipated fire sizes? In what locations are the fires expected to occur? If there are multiple possible fire types or locations, it is probably best to make them separate problems and address them one at a time.

At this stage, there should be a reasonably concise narrative description of the problem. The next step is to gather as much information as possible about the fuel and the geometry of the compartment(s). This should include the states of all doors and hatches and, if necessary, of the mechanical ventilation system. The latter is difficult to simulate with CFAST and is usually ignored. However, it may be very important for some problems and you may be forced to include ventilation effects. If so, it is suggested that the ventilation system be added after the rest of the model has been developed and successfully run. The primary reason for this recommendation is that development of the mechanical ventilation model is a time consuming, iterative process and it is pointless to perform this work until the underlying model has been completed.

After the problem has been clearly stated and the scenario has been accurately described, it is time to start building the actual model. The simplest case is that of a fire in a single compartment; therefore, it is highly recommended that the initial modeling effort be directed toward accurately defining the fire and the fire compartment. In the example discussed in this report, the fire compartment was a rectangular parallelepiped so the fire compartment geometry specification was trivial. In cases in which the fire compartment is complex, a reasonable approach is to start with a simple box having the same volume as the actual compartment, and concentrate on developing the most realistic fire specification possible. After this preliminary model has been successfully run, adjustments can then be made to improve the accuracy of the fire compartment geometry.

Once the model of the fire compartment is working, additional compartments may be added. It is suggested that this be done one compartment at a time, that the model be run after each addition and that any problems encountered by addressed immediately. Because the addition of a new compartment increments the number representing the exterior, it is important that the HVENT, VVENT and CFCON inputs be checked to ensure that the parameters are still correct after each addition. It is very helpful to make liberal use of comment lines to identify compartments by name, rather than by number, and to define the meaning of each parameter. Examples of the use of comments have been shown in the listings included in this report.

We have found that runtime problems are frequently associated with vent sizes (especially with the area specified by a VVENT input) and that the vent parameters may have to be adjusted in order to permit the model to run. The addition of a new compartment will sometimes lift pre-

existing restrictions so, after a new compartment has been added, it is advisable to revisit any previous alterations to determine whether they are still needed.

When the correct value of an input is not known (for example, the CO parameter) or when it is necessary to substitute an incorrect value (as was done with the VVENT area in our test case) in order for the model to run, it becomes very important to estimate the effects of this inaccuracy. The suggested method is to perform a sensitivity analysis by running the simulation with a range of input values. If possible, these inputs should bracket the entire range within which the actual value is expected to lie.

However, in some cases, such an analysis is not feasible. For example, when we initially attempted to apply the virtual compartment method to the Laundry Passageway model, we were unable to find a non-zero vertical vent area which did not cause CFAST to stall. Clearly, it was not possible to conduct a sensitivity analysis under these conditions. In this situation, an appropriate response is to reconsider the overall approach to the problem. In our example, we chose to use the compartment rearrangement, rather than the virtual compartment, technique.

Recall that CFAST has the ability to reduce the heat release rate in the event that it calculates that there is insufficient oxygen available. For this reason, it is useful to inspect the heat release rate output to verify that the model actually used the values that were specified. This need not be done after every change in inputs, but should be done (at least) after the model is complete. Note that deviations from the specified heat release rate are not necessarily incorrect – it is quite possible to specify a fire size that cannot be supported with the available oxygen supply. However, deviations should be investigated to rule out the possibility that they are artifacts of the simulation.

Time = 1208.0 seconds

Compartment	Upper Temp. (K)	Lower Temp. (K)	Inter. Height (m)	Pyrol Rate (kg/s)	Fire Size (W)	Pressure (Pa)	Ambient Target (W/m^2)
1	708.5	419.9	0.50	2.298E-02	9.598E+05	-4.45	1.156E+04
2	438.9	300.0	1.2	0.000E+00	0.000E+00	-0.849	585.
Outside	0.000E+00						

Table 9. CFAST Progress Update

A CFAST progress update, similar to this example, is displayed on the console device at an interval (in seconds) which specified by the second parameter associated with the TIMES keyword. If the F5 key is pressed while the model is running, the current simulation time and solver step size is appended to this output.

During execution, CFAST displays progress information (Table 9) on the default console device (most often, the computer monitor)[26] at user-specified intervals (set by the second parameter of the TIMES keyword). At typical CFAST execution speeds (better than 10 time faster than real time is common), these updates scroll very rapidly. However, they sometimes slow down drastically, indicating that the solver has made a bad guess regarding the step size. Normally, this problem is quickly corrected and CFAST resumes its usual, rapid execution. Our experience has

[26] The interval between progress updates (in seconds) is set by the second parameter of the TIMES keyword. Setting this parameter to zero suppresses updates; the default interval is one second.

been that, if the problem has not cleared within a few minutes, it may indicate a more serious stall. A good way to check this is to press the F5 key, which causes the current time and solver step size to be appended to the progress output, in the format "Time = xx.x, dt = yy." Step sizes (dt) of milliseconds or greater are typical of normal operation. Persistent sub-microsecond values are indicative of a stall. When this conditions occurs, we have found it best to kill the simulation, edit the input file to eliminate the cause of the stall and rerun the model.

In our case study, we relied on the CFAST capability for interpolating FMASS values between two specified endpoints. This interpolation capability also applies to some other inputs, such as the fractional opening of a horizontal vent (CVENT keyword), and is very useful in many cases. However, it can occasionally be the cause of problems. In particular, if the transition is too steep (*i.e.*, there is a large change in the parameter value between two closely spaced time points), CFAST may encounter numerical problems and drastically slow down or even stall. If problems of this nature are encountered, it is recommended that the transition be spread over a longer period of time.

If a step change is absolutely required, it may be possible to introduce it by using RESTR to initialize the simulation to values calculated by a previous simulation. For example, in previous work at NRL [3], it was desirable to instantaneously switch from a preburn period (a small pan fire) to a mass conflagration period (a large spray fire) at a specific time in the simulation. This was accomplished by simulating the pan fire, using the appropriate inputs, for the duration of the preburn. The model was then run again, with spray fire parameters, using the RESTR keyword to force the simulation to resume at the time of, and with the conditions that existed at, the end of the first run.

After the model results have been obtained, the obvious question will be: How good are the predictions? In our work, there was surprisingly good agreement between the model predictions and the SHADWELL/688 test results. In general, we have found that agreement tends to be best in and near the fire compartment (assuming that the fire was correctly defined) and progressively worse as the distance from the fire compartment increases, but we frequently have seen cases in which the predictions for one layer were very accurate and those for the other layer were not. In these cases, the upper layer is typically better than lower, possibly due to the absence, in CFAST, of mixing at the interface between layers.

However, it is important to understand that CFAST, like all similar models, is an engineering tool. Realistically, we can only expect CFAST to predict trends, not absolute values. In most cases, this is sufficient because it can be used to address one of the most common engineering questions: Is alternative A likely to be better or worse than B under the assumed conditions?

7.0 SUMMARY

We have demonstrated that, using CFAST, it is possible to build a model for a complex, multi-compartment shipboard fire scenario using the information that would be available to ship designers. In our first report [6], we showed that a fire specification could be created based largely on known or estimated fuel and combustion properties. Our second report [7] developed the geometrical specifications from a knowledge of the actual ship configuration. In this report, we have provided practical guidance to persons having a need to apply CFAST to shipboard fires. Due to the inherent limitations of the CFAST vocabulary, it is not possible to represent the details of many ship compartments. However, we have shown that it is possible to describe even complex fire scenarios using reasonable approximations.

For the fire, much of the necessary information is available in the literature or may be estimated from literature values. As an example of this process, we derived a value for the HCR input based on the fuel molecular weight and minimum hydrogen content. We found that two

parameters, OD and CO, cannot be accurately estimated from *a priori* knowledge. However, we have shown that, for OD, there is a saturation effect and that, as a result, many fires may be treated as either "clean" (no soot) or "dirty" (sooty). An OD value 0.06 appears to work very well for the latter case, which is the one of primary concern in Navy problems. We also demonstrated that the value for CO is often unimportant because it has very little effect on temperature or on the concentrations of carbon dioxide, soot or oxygen.

The techniques used for modeling of complex geometries included subdividing and rearranging compartments, using multiple virtual compartments to represent a single real compartment and adding dummy compartments. We also provided examples of methods for estimating mean values of thermophysical properties when compartment boundaries are composed of multiple patches of different materials.

We found that some situations could not be represented at all (for example, it is not possible for one compartment to simultaneously conduct heat through the overhead into two different compartments) and that specific combinations of input parameters could cause the CFAST to slow to the point of being effectively unusable. Because there is no known way to predict which input combinations will cause the latter problem or for what ranges of variables this problem will occur, we suggested a methodology for resolving stalling problems. This approach involved identification of the offending parameters by "commenting out" suspects, adjustment of the parameter values until the model runs successfully and fine tuning of the parameters to be as close to reality as possible without causing CFAST to stall.

It has been found to be very advantageous to build a complex model by starting with a simple, working case and adding features, one at a time, until the desired scenario is reached. When adding compartments to a model, feedback effects can significantly alter the behavior of pre-existing parts of the model. In some cases, the addition of a new compartment may permit the elimination of approximations that, in the absence of the new compartment, had been necessary.

8.0 ACKNOWLEDGMENTS

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Appendix A

CFAST Keywords Used in Modeling of the Submarine Ventilation Doctrine Configuration

VERSN	Version of CFAST for which the input file is intended. A title may also be specified for identification purposes.
TIMES	Simulation time and frequency of on-screen and file outputs.
DUMPR	Name of output file to be used.
FTIME	Event timeline.
RESTR	Name of restart fire, if any.

Table A-1. Simulation Control Keywords

TAMB	Internal ambient temperature, pressure and reference elevation.
EAMB	External ambient temperature, pressure and reference elevation.
WIND	Wind speed versus height parameters.

Table A-2. Ambient Environment Keywords

DEPTH	Depth (x-dimension) of the compartments, in meters. See FPOS.
WIDTH	Width (y-dimension) of the compartments, in meters. See FPOS.
HEIGH	Height (z-dimension) of the compartments, in meters. See FPOS.
HI/F	Floor elevation, relative to the reference elevation, in meters.
CEILI	Reference to an entry in the thermophysical properties database describing the ceilings.
WALLS	Reference to an entry in the thermophysical properties database describing the walls.
FLOOR	Reference to an entry in the thermophysical properties database describing the floors.
THRMF	Name of the thermophysical database to be used. If not specified, a default database, THERMAL.DF, is used.
HVENT	Definition of a horizontal vent, including the source and sink compartments, the vent number within the source compartment, the vent width and the heights of the soffit and sill.
VVENT	Definition of a vertical vent, including the source and sink compartments, the vent area and the shape (either round or square).
CVENT	Opening (width) of a horizontal vent as a fraction of the maximum width specified by the corresponding HVENT line.
CFCON	Enables vertical heat conduction through a ceiling to the floor of the compartment above.

Table A-3. Model Geometry Keywords

LFBO	Compartment number in which the main fire is located
FPOS	Coordinates (right-handed, Cartesian) of the fire location within the compartment relative to the lower, left, rear corner.
LFBT	Fire type. Type 1 is unconstrained by oxygen availability; type 2 is constrained.
FQDOT	Heat release rate of the burning fuel at the times specified by FTIME.
FMASS	Mass loss (pyrolysis) rate of the fuel at the times specified by FTIME
CHEMI	Miscellaneous parameters related to fuel combustion chemistry. Includes molecular weight and heat of combustion.
HCR	The mass ratio of hydrogen to carbon in the fuel.
O2	The mass ratio of available oxygen in the fuel to the total mass of fuel. This applies only to special cases, such as rocket fuels, in which the fuel consists o a mixture of oxidizing and reducing agents.
HCN	Ratio of the mass of HCN produced by pyrolysis to the mass of fuel pyrolyzed.
HCL	Ratio of the mass of HCl produced by pyrolysis to the mass of fuel pyrolyzed.
CT	Ratio of the mass of a virtual "total toxics" product to the mass of fuel pyrolyzed. This product is taken to be representative of the combined toxic effects of the actual pyrolysis and combustion products.
OD	Mass ratio of soot to carbon dioxide in the combustion products. This parameter is very important for correct prediction of temperatures (reference [4]).
CO	Mass ratio of carbon monoxide to carbon dioxide in the combustion products.
FHIGH	Height of the base of the fire (above the reference position established by FPOS) at the times specified by FTIME.
FAREA	Horizontal area of the base of the fire at the times specified by FTIME.
CJET	Switches between the "standard" and "ceiling jet" model of convective heat transfer to the ceiling.

Table A-4. Fire Description Keywords